

Conserving Gapless Mean-Field Theory for Weakly Interacting Bose Gases

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This paper presents a conserving gapless mean-field theory for weakly interacting Bose gases. We first construct a mean-field Luttinger-Ward thermodynamic functional in terms of the condensate wave function Ψ and the Nambu Green's function \hat{G} for the quasiparticle field. Imposing its stationarity respect to Ψ and \hat{G} yields a set of equations to determine the equilibrium for general non-uniform systems. They have a plausible property of satisfying the Hugenholtz-Pines theorem to provide a gapless excitation spectrum. Also, the corresponding dynamical equations of motion obey various conservation laws. Thus, the present mean-field theory shares two important properties with the exact theory: “conserving” and “gapless.” The theory is then applied to a homogeneous weakly interacting Bose gas with s -wave scattering length a and particle mass m to clarify its basic thermodynamic properties under two complementary conditions of constant density n and constant pressure p . The superfluid transition is predicted to be first-order because of the non-analytic nature of the order-parameter expansion near T_c inherent in Bose systems, i.e., the Landau-Ginzburg expansion is not possible here. The transition temperature T_c shows quite a different interaction dependence between the n -fixed and p -fixed cases. In the former case T_c increases from the ideal gas value T_0 as $T_c/T_0 = 1 + 2.33an^{1/3}$, whereas it decreases in the latter as $T_c/T_0 = 1 - 3.84a(mp/2\pi\hbar^2)^{1/5}$. Temperature dependences of basic thermodynamic quantities are clarified explicitly.

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I. INTRODUCTION

Mean-field theories with self-consistency equations have played a central role in the development of our microscopic understanding on quantum many-particle systems, especially on broken-symmetry phases. One of the most outstanding examples is undoubtedly the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity,¹ which may be regarded now as the Hartree-Fock theory in the Nambu space.² In some notable cases like the BCS theory, mean-field theories have brought remarkable quantitative descriptions of experiments. At least, each mean-field theory have provided a basic starting point for later developments, as the Weiss³ and the Stoner⁴ theories for localized and itinerant ferromagnets, respectively. Hence there is every need for a mean-field theory of every quantum system. However, there has been no established mean-field theory for Bose-Einstein condensates (BEC).

Over the last sixty years, the field theory has manifested itself as one of the most powerful microscopic approaches to quantum many-particle systems. It was first applied to Bose particles in the celebrated work of Bogoliubov,⁵ followed by intensive theoretical investigations in later years.^{6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30} However, it has brought a rather poor description of condensed Bose particles at finite temperatures. For example, we still do not have a complete agreement on the Bose-Einstein condensation temperature T_c of the homogeneous weakly interacting Bose gas under constant density n ,^{31,32,33,34,35,36,37,38,39,40,41,42,43} not to mention its thermodynamic properties over $0 \leq T \leq T_c$; see Refs. 42 and 43 for a review on the T_c calculations. This situation is partly due to the absence of

a well-established renormalized perturbation theory for Bose systems corresponding to the Luttinger-Ward theory on Fermi liquids.⁴⁴ Indeed, important formal results on Bose systems have often been obtained with the bare perturbation theory, as in the case of the Hugenholtz-Pines theorem.¹⁶ However, the bare perturbation expansion itself is not very suitable for practical calculations due to the infrared divergences inherent in Bose systems. On the other hand, we still do not have a systematic approximation scheme of how to renormalize the condensate wave function and the quasiparticle Green's function self-consistently without losing the physical essentials of condensed Bose particles.

The self-consistent Wick decomposition procedure has proved to be quite powerful for most quantum many-particle systems at finite temperatures and might be used also for Bose particles. The corresponding mean-field theory for condensed Bose systems is known now as the Girardeau-Arnouitt theory^{14,25} or the Hartree-Fock-Bogoliubov (HFB) theory.⁴⁵ However, it predicts an energy gap in the excitation spectrum, in contradiction to the Hugenholtz-Pines theorem of declaring a gapless excitation. Thus, it has become customary to introduce a further approximation to the HFB theory, now generally called the “Popov” approximation,⁴⁵ of completely ignoring the anomalous quasiparticle pair correlation to recover a gapless excitation. When it is adopted to describe dynamics, however, the same approximation does not satisfy various conservation laws as required. Also, it is not clear whether it is permissible or not to neglect the pair correlation completely. Recently, Proukakis *et al.*⁴⁶ have presented an improved gapless theory with finite pair correlation. However, it still does not satisfy the conservation laws. Thus, there has been no mean-field theory for condensed Bose systems that simultane-

ously carries the important properties of the exact theory pointed out by Hohenberg and Martin:²⁵ “conserving” and “gapless.”

On the basis of these observations, we have recently formulated a new mean-field theory for BEC with the desired conserving gapless character.⁴⁷ We here present a detailed description of the theory with several new results. As first shown by Baym for normal Fermi liquids⁴⁸ and pointed out by Hohenberg and Martin for condensed Bose systems,²⁵ various conservation laws are automatically satisfied in the “ Φ derivative approximations” where the irreducible self-energy $\hat{\Sigma}$ is obtained as a derivative of some functional $\Phi = \Phi[\hat{G}]$ with respect to the renormalized Green’s function \hat{G} . This relationship between $\hat{\Sigma}$ and \hat{G} holds exactly for Fermi systems in equilibrium, as shown by Luttinger and Ward.⁴⁴ Indeed, Φ was first introduced by Luttinger and Ward as part of the exact thermodynamic functional $\Omega = \Omega[\hat{G}]$. It was later taken up by Baym⁴⁸ to present a criterion for obtaining approximate dynamical equations with conservation laws. It thus follows that dynamical equations obtained from a Luttinger-Ward functional naturally obey the conservation laws. We hence ask the heuristic question here: Can we construct a mean-field Luttinger-Ward thermodynamic functional for BEC that also satisfies the Hugenholtz-Pines theorem? This is indeed possible as will be shown below. The predictions of the resulting mean-field theory on the homogeneous weakly interacting Bose gas will be presented later with an expression for ΔT_c ; this application hopefully will provide a deeper insight into the superfluidity and phase transition of still mysterious ^4He .^{49,50} It should be noted that the same idea has been adopted more recently by Ivanov, Riek, and Knoll⁵¹ (IRK) in a different context of the $O(N)$ model to present an apparently different thermodynamic functional. It will be shown, however, that their functional yields exactly the same equilibrium thermodynamic properties on weakly interacting Bose gases as the present one.

We finally provide three comments on terminology to remove possible confusions in advance. First, Gardiner⁵² and Castin and Dum⁵³ have presented an alternative description of BEC, which was called by Gardiner⁵² as “particle-number conserving Bogoliubov method.” However, his terminology is completely different from the present “conserving” and we call their formulations as “number-fixed” descriptions of BEC. Indeed, his terminology is connected more closely with the equilibrium thermodynamics to denote the fact that the particle number N is chosen as an independent variable instead of the chemical potential μ . The two descriptions of using N and μ are equivalent in the thermodynamic limit except the fluctuation in the particle number. It is worth pointing out that a “number-fixed” theory does not necessarily provide “conserving” dynamical equations in the present sense. Second, the term “gapless” is relevant here to the single-particle excitation. Indeed, the collective excitation has another story and is gapless even

in the Girardeau-Arnouitt theory, as already shown by Takano.¹⁸ Third, it has been pointed out by Yukalov⁴³ that the word “Popov” may not be suitable for the approximation of setting the anomalous pair amplitude equal to zero in the HFB theory. Indeed, this approximation was introduced by Shohn²² already in 1964 and used later by Reatto and Straley.²⁹ We can also find the same approximation later in the work of Baym and Grinstein on the σ model.⁵⁴ We will call it as the “Shohn” approximation instead of “Popov” following Reatto and Straley.²⁹

This paper is organized as follows. Section II presents a mean-field free-energy functional for general non-uniform systems and derives a closed set of equations to determine the thermodynamic equilibrium. Section III applies the formulation to the homogeneous weakly interacting Bose gas under constant density to clarify its basic thermodynamic properties. Section IV treats the same system under the complementary condition of constant pressure. Section V concludes the paper. Appendix A summarizes Feynman rules for the perturbation expansion with respect to the Nambu Green’s function. Appendix B provides a proof on the condensed Bose systems that the conservation laws are obeyed in the Φ derivative approximations. In Appendix C, the connection between the present and the IRK theories is clarified. Appendix D discusses the origin of a non-Hermitian eigenvalue problem in condensed Bose systems. Appendix E derives compact expressions for the equilibrium thermodynamic functional and the entropy. We put $k_B = 1$ throughout.

II. MEAN-FIELD EQUATIONS

A. Free-energy functional

We express the field operator $\psi(\mathbf{r})$ as a sum of the condensate wave function $\Psi(\mathbf{r})$ and the quasiparticle field $\phi(\mathbf{r})$ as

$$\psi(\mathbf{r}) = \Psi(\mathbf{r}) + \phi(\mathbf{r}). \quad (1)$$

It is convenient to introduce the spinors:

$$\vec{\phi} \equiv \begin{bmatrix} \phi \\ \phi^\dagger \end{bmatrix}, \quad \vec{\phi}^\dagger \equiv [\phi^\dagger \ \phi], \quad (2a)$$

$$\vec{\Psi} \equiv \begin{bmatrix} \Psi \\ \Psi^* \end{bmatrix}, \quad \vec{\Psi}^\dagger \equiv [\Psi^* \ \Psi]. \quad (2b)$$

Using Eq. (2a), we define our Matsubara Green’s function in Nambu space² as

$$\begin{aligned} \hat{G}(\mathbf{r}, \mathbf{r}'; \tau) &\equiv -\hat{\tau}_3 \langle T_\tau \vec{\phi}(\mathbf{r}, \tau) \vec{\phi}^\dagger(\mathbf{r}') \rangle \\ &= T \sum_{n=-\infty}^{\infty} \hat{G}(\mathbf{r}, \mathbf{r}'; z_n) e^{-z_n \tau}, \end{aligned} \quad (3)$$

with $\hat{\tau}_3$ the third Pauli matrix and $z_n \equiv 2\pi i n T$. The factor $\hat{\tau}_3$ is usually absent in the definition of Green's function.^{25,45} Introducing the factor brings an advantage that the eigenvalue problem for \hat{G}^{-1} is equivalent to the Bogoliubov-de Gennes (BdG) equation for the quasiparticles, as seen below. Thus, \hat{G} can be put into a diagonal form with respect to the eigenstates of the BdG equation.

The bare perturbation expansion for condensed Bose systems may also be performed quite compactly in terms of the Nambu-Matsubara Green's function of Eq. (3). The corresponding Feynman rules can be found easily from those of the superconducting Fermi systems⁵⁵ with slight modifications, which are summarized in Appendix A. Retaining the lowest-order diagrams in terms of the interaction and renormalizing $\hat{G}_0 \rightarrow \hat{G}$, one may express the free-energy functional of the HFB theory in a Luttinger-Ward form^{44,55} with respect to Ψ and \hat{G} .

We now present our mean-field Luttinger-Ward functional $\Omega = \Omega(\Psi, \Psi^*, \hat{G})$ which has been obtained from that of the HFB theory with a slight modification. It is given by

$$\Omega = \int \Psi^*(\mathbf{r}) K \Psi(\mathbf{r}) d\mathbf{r} + \frac{T}{2} \sum_n \text{Tr} \left[\ln(\hat{\tau}_3 K + \hat{\Sigma} - z_n \hat{1}) + \hat{G} \hat{\Sigma} \right] \hat{1}(z_n) + \Phi. \quad (4)$$

Here K is defined by

$$K \equiv -\frac{\hbar^2}{2m} \nabla^2 + \mathcal{V}(\mathbf{r}) - \mu_s, \quad (5)$$

with $\mathcal{V}(\mathbf{r})$ the external potential and μ_s the chemical potential, $\hat{1}$ is the unit matrix, and $\hat{1}(z_n)$ denotes

$$\hat{1}(z_n) = \begin{bmatrix} e^{z_n 0_+} & 0 \\ 0 & e^{-z_n 0_+} \end{bmatrix}, \quad (6)$$

with 0_+ an infinitesimal positive constant. The branch cut of the logarithm in Eq. (4) is chosen along the negative real axis, and Tr here includes an integration over space variables with multiplications of $\hat{\tau}_3 K$ and $-z_n \hat{1}$ by $\delta(\mathbf{r} - \mathbf{r}')$ from the right implied. Finally, $\hat{\Sigma}$ denotes the irreducible self-energy obtained from the functional $\Phi = \Phi(\Psi, \Psi^*, \hat{G})$ by

$$\hat{\Sigma}(\mathbf{r}, \mathbf{r}'; z_n) = -\frac{2}{T} \frac{\delta \Phi}{\delta \hat{G}(\mathbf{r}', \mathbf{r}; z_n)}. \quad (7)$$

With Eq. (7), Ω becomes stationary with respect to a variation in \hat{G} satisfying Dyson's equation:

$$\hat{G}^{-1} = z_n \hat{1} - \hat{\tau}_3 K - \hat{\Sigma}. \quad (8)$$

The condensate wave function $\Psi(\mathbf{r})$ in equilibrium is also determined by $\delta \Omega / \delta \Psi^*(\mathbf{r}) = 0$. Noting $\delta \Omega / \delta \hat{G} = \hat{0}$, we only need to consider the explicit Ψ^* dependences in Ω to obtain

$$K \Psi(\mathbf{r}) = -\eta(\mathbf{r}), \quad (9)$$

with

$$\eta(\mathbf{r}) \equiv \frac{\delta \Phi}{\delta \Psi^*(\mathbf{r})}. \quad (10)$$

The quantity $\eta(\mathbf{r})$ is the so-called condensate source function.^{25,45} Equations (7) and (10) constitute the Φ derivative approximation²⁵ where the conservation laws are obeyed automatically by the dynamical equations. This is one of the main advantages in using the Luttinger-Ward functional as a starting point.

Despite their importance, the conservation laws in the Φ -derivative approximation seems not to have been described to an enough extent in the literature for the condensed Bose systems. We hence provide a detailed proof of them in Appendix B.

A key quantity in Eq. (4) is Φ . We choose it so that the Hugenholtz-Pines theorem is satisfied simultaneously. Explicitly, it is given by

$$\begin{aligned} \Phi = & \int d\mathbf{r} \int d\mathbf{r}' \mathcal{U}(\mathbf{r} - \mathbf{r}') \left[\frac{1}{2} |\Psi(\mathbf{r})|^2 |\Psi(\mathbf{r}')|^2 \right. \\ & - \frac{T}{2} \sum_n |\Psi(\mathbf{r})|^2 \text{Tr} \hat{\tau}_3 \hat{G}(\mathbf{r}', \mathbf{r}'; z_n) \hat{1}(z_n) \\ & - \frac{T}{2} \sum_n \text{Tr} \hat{\tau}_3 \vec{\Psi}(\mathbf{r}) \vec{\Psi}^\dagger(\mathbf{r}') \hat{G}(\mathbf{r}', \mathbf{r}; z_n) \hat{1}(z_n) \\ & + \frac{T^2}{8} \sum_{n, n'} \text{Tr} \hat{\tau}_3 \hat{G}(\mathbf{r}, \mathbf{r}, z_n) \hat{1}(z_n) \text{Tr} \hat{\tau}_3 \hat{G}(\mathbf{r}', \mathbf{r}'; z_{n'}) \hat{1}(z_{n'}) \\ & \left. + \frac{T^2}{4} \sum_{n, n'} \text{Tr} \hat{G}(\mathbf{r}, \mathbf{r}'; z_n) \hat{1}(z_n) \hat{G}(\mathbf{r}', \mathbf{r}; z_{n'}) \hat{1}(z_{n'}) \right], \quad (11a) \end{aligned}$$

where \mathcal{U} denotes the interaction potential. As may be realized from Appendix A where the Feynman rules in Nambu space are given explicitly, the five terms in the square brackets of Eq. (11a) corresponds to the diagrams of Fig. 1(a)-(e), respectively. The difference of Eq. (11a) from Φ_{HFB} lies in the Fock terms, i.e., the third and the fifth terms. Indeed, Φ_{HFB} ^{25,45} is recovered from Eq. (11a) by replacing \hat{G} and $\hat{\tau}_3 \vec{\Psi}(\mathbf{r}) \vec{\Psi}^\dagger(\mathbf{r}')$ in the two Fock terms by $\hat{\tau}_3 \hat{G}$ and $\vec{\Psi}(\mathbf{r}) \vec{\Psi}^\dagger(\mathbf{r}')$, respectively; the present functional was found in the reverse way.

At this stage, it may be worth providing a comment on the present functional. As mentioned by Shi and Griffin,⁵⁶ the HFB approximation yields over-counting of the off-diagonal self-energy diagrams in the bare perturbation expansion, thereby leading to an unphysical energy gap in the excitation spectrum. Hence it is necessary to subtract the extra contributions from the HFB self-energy. In this context, it is interesting to note that the present functional removes some of the off-diagonal terms in Φ_{HFB} as

$$\begin{aligned} \Phi = & \Phi_{\text{HFB}} - \int d\mathbf{r} \int d\mathbf{r}' \mathcal{U}(\mathbf{r} - \mathbf{r}') [\Psi(\mathbf{r}) \Psi(\mathbf{r}') \langle \phi^\dagger(\mathbf{r}') \phi^\dagger(\mathbf{r}) \rangle \\ & + \Psi^*(\mathbf{r}) \Psi^*(\mathbf{r}') \langle \phi(\mathbf{r}') \phi(\mathbf{r}) \rangle + |\langle \phi(\mathbf{r}) \phi(\mathbf{r}') \rangle|^2]. \quad (11b) \end{aligned}$$

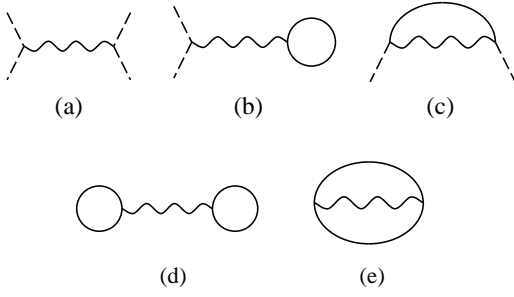


FIG. 1: Diagrams contributing to Φ . The wavy, the solid, and the broken lines denote the interaction, the Nambu Green's function, and the condensate wave function, respectively.

It satisfies the Hugenholtz-Pines relation appropriately to be free from the unphysical excitation gap, as seen below. Thus, the subtraction mentioned above may have been performed appropriately.

Based on exactly the same idea as adopted here, Ivanov, Riek, and Knoll⁵¹ have recently constructed an alternative functional Φ_{IRK} for the $O(N)$ model so as to satisfy the Hugenholtz-Pines theorem. Their functional is given in the present context by

$$\Phi_{\text{IRK}} = \Phi_{\text{HFB}} - \int d\mathbf{r} \int d\mathbf{r}' \mathcal{U}(\mathbf{r}-\mathbf{r}') |\langle \phi(\mathbf{r}) \phi(\mathbf{r}') \rangle|^2. \quad (12)$$

In spite of the apparent difference between Eqs. (11b) and (12), however, Φ and Φ_{IRK} lead to exactly the same thermodynamic properties for weakly interacting Bose gases, as shown in Appendix C.

B. Equilibrium solution

Now that Φ is given explicitly, we obtain the equilibrium self-energy by Eq. (7). It may be written as

$$\hat{\Sigma}(\mathbf{r}, \mathbf{r}') = \begin{bmatrix} \Sigma(\mathbf{r}, \mathbf{r}') & \Delta(\mathbf{r}, \mathbf{r}') \\ -\Delta^*(\mathbf{r}, \mathbf{r}') & -\Sigma^*(\mathbf{r}, \mathbf{r}') \end{bmatrix}, \quad (13)$$

where Σ and Δ are given by

$$\begin{aligned} \Sigma(\mathbf{r}, \mathbf{r}') &= \delta(\mathbf{r}-\mathbf{r}') \int d\mathbf{r}'' \mathcal{U}(\mathbf{r}-\mathbf{r}'') \rho(\mathbf{r}'', \mathbf{r}'') d\mathbf{r}'' \\ &\quad + \mathcal{U}(\mathbf{r}-\mathbf{r}') \rho(\mathbf{r}, \mathbf{r}'), \end{aligned} \quad (14a)$$

$$\Delta(\mathbf{r}, \mathbf{r}') = \mathcal{U}(\mathbf{r}-\mathbf{r}') \tilde{\rho}(\mathbf{r}, \mathbf{r}'), \quad (14b)$$

respectively, with

$$\rho(\mathbf{r}, \mathbf{r}') = \Psi(\mathbf{r}) \Psi^*(\mathbf{r}') + \langle \phi^\dagger(\mathbf{r}') \phi(\mathbf{r}) \rangle, \quad (15a)$$

$$\tilde{\rho}(\mathbf{r}, \mathbf{r}') = \Psi(\mathbf{r}) \Psi(\mathbf{r}') + \langle \phi(\mathbf{r}) \phi(\mathbf{r}') \rangle. \quad (15b)$$

The equation for the condensate wave function in equilibrium is obtained from Eqs. (9), (10), and (11a). It can be written explicitly in terms of Eq. (14) by

$$K\Psi(\mathbf{r}) + \int [\Sigma(\mathbf{r}, \mathbf{r}') \Psi(\mathbf{r}') - \Delta(\mathbf{r}, \mathbf{r}') \Psi^*(\mathbf{r}')] d\mathbf{r}' = 0. \quad (16)$$

In the homogeneous case with no external potential where $K \rightarrow -\mu_s$ and $\Psi = \sqrt{n_0}$ with n_0 the condensate density, Eq. (16) reduces to the Hugenholtz-Pines relation $\mu_s = \Sigma_{\mathbf{k}=\mathbf{0}} - \Delta_{\mathbf{k}=\mathbf{0}}$, as desired. The expression for the particle number $N = -\partial\Omega/\partial\mu_s$ is found similarly as

$$N = \int \rho(\mathbf{r}, \mathbf{r}) d\mathbf{r}, \quad (17)$$

with ρ given by Eq. (15a). Using this equation, one may change independent variables of the free energy as $\Omega(T, V, \mu) \rightarrow F(T, V, N) \equiv \Omega(T, V, \mu) + \mu N$. Equations (8) and (13)-(17) determines the equilibrium.

C. Bogoliubov-de Gennes equations

Physical quantities in equilibrium may be calculated most conveniently in the representation where \hat{G} is diagonal. Noting Eq. (8), we introduce

$$\hat{H}(\mathbf{r}, \mathbf{r}') \equiv \hat{\tau}_3 K \delta(\mathbf{r}-\mathbf{r}') + \hat{\Sigma}(\mathbf{r}, \mathbf{r}'). \quad (18)$$

The eigenvalue problem for \hat{H} constitutes the BdG equation:

$$\int \hat{H}(\mathbf{r}, \mathbf{r}') \vec{\varphi}_\mu(\mathbf{r}') d\mathbf{r}' = E_\mu \vec{\varphi}_\mu(\mathbf{r}), \quad (19a)$$

where $\vec{\varphi}_\mu$ denotes an eigenfunction. It has a peculiar feature that \hat{H} is not Hermitian but satisfies $\hat{H}^\dagger(\mathbf{r}, \mathbf{r}') = \hat{\tau}_3 \hat{H}(\mathbf{r}', \mathbf{r}) \hat{\tau}_3$. Since most of the eigenvalue problems in quantum mechanics are Hermitian by nature, it may be worth tracing why we have to treat a non-Hermitian matrix in BEC. It is shown in Appendix D that this symmetry necessarily results from the requirement that the quasiparticle field obey the Bose statistics.

Let us enumerate basic properties of the BdG equation, since this seems not to have been performed to an enough extent in the literature. We will also provide a compact Nambu representation to every quantity of the BdG equation. Taking its Hermitian conjugate and using $\hat{H}^\dagger(\mathbf{r}, \mathbf{r}') = \hat{\tau}_3 \hat{H}(\mathbf{r}', \mathbf{r}) \hat{\tau}_3$, Eq. (19a) may be written alternatively as

$$\int \vec{\varphi}_{\mu'}^\dagger(\mathbf{r}) \hat{\tau}_3 \hat{H}(\mathbf{r}, \mathbf{r}') \hat{\tau}_3 d\mathbf{r} = E_{\mu'}^* \vec{\varphi}_{\mu'}^\dagger(\mathbf{r}'). \quad (19b)$$

Let us multiply Eq. (19a) by $\vec{\varphi}_{\mu'}^\dagger(\mathbf{r}) \hat{\tau}_3$ from the left and integrate it over \mathbf{r} . Similarly, we multiply Eq. (19b) by $\hat{\tau}_3 \vec{\varphi}_\mu(\mathbf{r}')$ from the right and integrate it over \mathbf{r}' . Subtracting the latter from the former, we obtain

$$(E_\mu - E_{\mu'}^*) \langle \vec{\varphi}_{\mu'} | \hat{\tau}_3 | \vec{\varphi}_\mu \rangle = 0. \quad (20)$$

We first put $\mu' = \mu$ in Eq. (20). We then realize that E_μ is real as long as $\langle \vec{\varphi}_\mu | \hat{\tau}_3 | \vec{\varphi}_\mu \rangle \neq 0$ can be satisfied by the eigenstate. We assume that (i) this is the case and (ii) eigenstates with positive eigenvalues may be normalized as $\langle \vec{\varphi}_\mu | \hat{\tau}_3 | \vec{\varphi}_\mu \rangle = 1$. We next consider the case $E_{\mu'} \neq E_\mu$ in Eq. (20). We then find that the two eigenstates with different eigenvalues are orthogonal as $\langle \vec{\varphi}_{\mu'} | \hat{\tau}_3 | \vec{\varphi}_\mu \rangle = 0$.

The Hamiltonian \hat{H} has another symmetry: $\hat{H}(\mathbf{r}, \mathbf{r}') = -\hat{\tau}_1 \hat{H}^*(\mathbf{r}, \mathbf{r}') \hat{\tau}_1$ with $\hat{\tau}_1$ the first Pauli matrix. Let us take the complex conjugate of Eq. (19a), multiply it by $-\hat{\tau}_1$ from the left, and use the above symmetry. It is thereby shown that a positive eigenvalue E_ν of the BdG equation with the eigenfunction:

$$\vec{u}_\nu(\mathbf{r}) \equiv \begin{bmatrix} u_\nu(\mathbf{r}) \\ -v_\nu^*(\mathbf{r}) \end{bmatrix}, \quad (21a)$$

is always accompanied by the negative eigenvalue $-E_\nu$ with the eigenfunction:

$$\vec{v}_\nu(\mathbf{r}) \equiv \begin{bmatrix} -v_\nu(\mathbf{r}) \\ u_\nu^*(\mathbf{r}) \end{bmatrix}. \quad (21b)$$

The sign in front of v_ν^* is introduced for convenience to make the coefficient $v_{\mathbf{k}}$ of the homogeneous system positive. As mentioned above, we assume that $\vec{u}_\nu(\mathbf{r})$ with $E_\nu > 0$ can be normalized as

$$\langle u_\nu | u_\nu \rangle - \langle v_\nu | v_\nu \rangle = 1. \quad (21c)$$

Violation of this condition marks an instability of the assumed $\Psi(\mathbf{r})$, as is the case of a vortex-free $\Psi(\mathbf{r})$ under an angular velocity Ω beyond the critical value Ω_{c1} .

It also follows from Eq. (16) that the BdG equation has eigenvalue 0 whose eigenfunction is proportional to $\hat{\tau}_3 |\vec{\Psi}\rangle$ with $|\vec{\Psi}\rangle$ given by Eq. (2b). We adopt the following normalized eigenfunction for this state:

$$\vec{\varphi}_0^{(1)}(\mathbf{r}) \equiv \frac{1}{\langle \vec{\Psi} | \vec{\Psi} \rangle^{1/2}} \hat{\tau}_3 \vec{\Psi}(\mathbf{r}) = \begin{bmatrix} \varphi_0(\mathbf{r}) \\ -\varphi_0^*(\mathbf{r}) \end{bmatrix}. \quad (22a)$$

It is orthogonal to $|\vec{u}_\nu\rangle$ as $\langle \vec{u}_\nu | \hat{\tau}_3 | \vec{\varphi}_0^{(1)} \rangle = 0$, i.e., $\langle u_\nu | \varphi_0 \rangle = \langle \varphi_0 | v_\nu \rangle$. Noting Eq. (21c), we may assume

$$\langle u_\nu | \varphi_0 \rangle = \langle v_\nu | \varphi_0 \rangle = 0. \quad (22b)$$

There still remains another independent state:

$$\vec{\varphi}_0^{(2)}(\mathbf{r}) \equiv \hat{\tau}_3 \vec{\varphi}_0^{(1)}(\mathbf{r}) = \begin{bmatrix} \varphi_0(\mathbf{r}) \\ \varphi_0^*(\mathbf{r}) \end{bmatrix}, \quad (22c)$$

which does not belong to \hat{H} , however. The functions $\vec{\varphi}_0^{(j)}(\mathbf{r})$ ($j=1, 2$) satisfy $\langle \vec{\varphi}_0^{(i)} | \hat{\tau}_3 | \vec{\varphi}_0^{(j)} \rangle = 1 - \delta_{ij}$.

The functions $|\vec{u}_\nu\rangle$, $|\vec{v}_\nu\rangle$, $|\vec{\varphi}_0^{(1)}\rangle$, and $|\vec{\varphi}_0^{(2)}\rangle$ are assumed to form a complete set. As shown by expanding an arbitrary spinor with respect to the basis functions and calculating the corresponding expansion coefficients, this statement is equivalent to

$$\begin{aligned} & \sum_\nu (|\vec{u}_\nu\rangle \langle \vec{u}_\nu | \hat{\tau}_3 - |\vec{v}_\nu\rangle \langle \vec{v}_\nu | \hat{\tau}_3) \\ & + |\vec{\varphi}_0^{(1)}\rangle \langle \vec{\varphi}_0^{(2)} | \hat{\tau}_3 + |\vec{\varphi}_0^{(2)}\rangle \langle \vec{\varphi}_0^{(1)} | \hat{\tau}_3 = \hat{1}. \end{aligned} \quad (23)$$

In summary, the BdG equation for a pair of eigenstates $\pm E_\nu$ ($E_\nu > 0$) can be written compactly in a matrix form as

$$\int \hat{H}(\mathbf{r}, \mathbf{r}') \hat{u}_\nu(\mathbf{r}') d\mathbf{r}' = \hat{u}_\nu(\mathbf{r}) E_\nu \hat{\tau}_3, \quad (24)$$

where \hat{u}_ν is defined by

$$\hat{u}_\nu(\mathbf{r}) = \begin{bmatrix} u_\nu(\mathbf{r}) & -v_\nu(\mathbf{r}) \\ -v_\nu^*(\mathbf{r}) & u_\nu^*(\mathbf{r}) \end{bmatrix}. \quad (25a)$$

There exists another independent state composed of the condensate wave function $\Psi(\mathbf{r})$:

$$\hat{\varphi}_0(\mathbf{r}) = \begin{bmatrix} \varphi_0(\mathbf{r}) & \varphi_0(\mathbf{r}) \\ -\varphi_0^*(\mathbf{r}) & \varphi_0^*(\mathbf{r}) \end{bmatrix}, \quad \varphi_0(\mathbf{r}) = \frac{1}{\sqrt{2N_0}} \Psi(\mathbf{r}), \quad (25b)$$

with $N_0 \equiv \frac{1}{2} \langle \vec{\Psi} | \vec{\Psi} \rangle$ denoting the condensate number. The orthonormality of the basis functions reads

$$\int \hat{\tau}_3 \hat{u}_\nu^\dagger(\mathbf{r}) \hat{\tau}_3 \hat{u}_{\nu'}(\mathbf{r}) d\mathbf{r} = \delta_{\nu\nu'} \hat{1}, \quad (26a)$$

$$\int \hat{\tau}_1 \hat{\varphi}_0^\dagger(\mathbf{r}) \hat{\tau}_3 \hat{\varphi}_0(\mathbf{r}) d\mathbf{r} = \hat{1}, \quad (26b)$$

$$\int \hat{\tau}_3 \hat{u}_\nu^\dagger(\mathbf{r}) \hat{\tau}_3 \hat{\varphi}_0(\mathbf{r}) d\mathbf{r} = \hat{0}. \quad (26c)$$

The completeness (23) can be written alternatively as

$$\sum_\nu \hat{u}_\nu(\mathbf{r}) \hat{\tau}_3 \hat{u}_\nu^\dagger(\mathbf{r}') \hat{\tau}_3 + \hat{\varphi}_0(\mathbf{r}) \hat{\tau}_1 \hat{\varphi}_0^\dagger(\mathbf{r}') \hat{\tau}_3 = \delta(\mathbf{r} - \mathbf{r}') \hat{1}, \quad (27)$$

as seen by writing down the matrix elements explicitly.

Equations (24)-(27) are the basic properties of the eigenstates of the BdG equation. Noting that $\vec{\varphi}_0^{(2)}(\mathbf{r})$ is absent in \hat{H} , Eq. (18) may be expanded as

$$\hat{H}(\mathbf{r}, \mathbf{r}') = \sum_\nu \hat{u}_\nu(\mathbf{r}) E_\nu \hat{\tau}_3 \hat{u}_\nu^\dagger(\mathbf{r}') \hat{\tau}_3. \quad (28)$$

Green's function $\hat{G} = (z_n \hat{1} - \hat{H})^{-1}$ becomes diagonal in the representation where \hat{H} is. In addition, eigenvalue 0 is absent in \hat{G} . Hence $\hat{G}(\mathbf{r}, \mathbf{r}'; z_n)$ can be written as

$$\hat{G}(\mathbf{r}, \mathbf{r}'; z_n) = \sum_\nu \hat{u}_\nu(\mathbf{r}) \hat{G}_\nu(z_n) \hat{\tau}_3 \hat{u}_\nu^\dagger(\mathbf{r}') \hat{\tau}_3, \quad (29a)$$

with

$$\hat{G}_\nu(z_n) = \begin{bmatrix} (z_n - E_\nu)^{-1} & 0 \\ 0 & (z_n + E_\nu)^{-1} \end{bmatrix}. \quad (29b)$$

Substituting Eq. (29) into Eq. (3) and performing summation over z_n with $\tau = -0_+$, we obtain the expressions for $\langle \phi^\dagger(\mathbf{r}') \phi(\mathbf{r}) \rangle$ and $\langle \phi(\mathbf{r}) \phi(\mathbf{r}') \rangle$ as

$$\langle \phi^\dagger(\mathbf{r}') \phi(\mathbf{r}) \rangle = \sum_\nu [u_\nu(\mathbf{r}) u_\nu^*(\mathbf{r}') n_\nu + v_\nu(\mathbf{r}) v_\nu^*(\mathbf{r}') (1 + n_\nu)], \quad (30a)$$

$$\langle \phi(\mathbf{r})\phi(\mathbf{r}') \rangle = \frac{1}{2} \sum_{\nu} [u_{\nu}(\mathbf{r})v_{\nu}(\mathbf{r}') + v_{\nu}(\mathbf{r})u_{\nu}(\mathbf{r}')] (1 + 2n_{\nu}), \quad (30b)$$

where $n_{\nu} \equiv (e^{E_{\nu}/T} - 1)^{-1}$ is the Bose distribution function, and we have used the (1, 2) element of Eq. (27) to make Eq. (30b) manifestly symmetric with respect to \mathbf{r} and \mathbf{r}' .

Equations (14)-(18), (24), and (30) form a closed set of self-consistent equations satisfying both the Hugenholtz-Pines theorem and various conservation laws. Note that the pair correlation $\langle \phi\phi \rangle$ is adequately included in Eqs. (16) and (24); neglecting this contribution yields the Shohno theory.²²

D. Expressions of equilibrium

It is shown in Appendix E that we can transform Eq. (4) in equilibrium into

$$\Omega_{\text{eq}} = T \sum_{\nu} \ln(1 - e^{-E_{\nu}/T}) - \sum_{\nu} E_{\nu} \int |v_{\nu}(\mathbf{r})|^2 d\mathbf{r} - \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' [\Sigma(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}', \mathbf{r}) - \Delta^*(\mathbf{r}, \mathbf{r}')\tilde{\rho}(\mathbf{r}', \mathbf{r})]. \quad (31)$$

The entropy in equilibrium can be obtained from $S_s = -\partial\Omega/\partial T$ by differentiating Eq. (4) in terms of the explicit T dependences. As shown in Appendix E, this yields

$$S_s = \sum_{\nu} [(1 + n_{\nu}) \ln(1 + n_{\nu}) - n_{\nu} \ln n_{\nu}]. \quad (32)$$

This completes the formulation of our mean-field theory.

III. HOMOGENEOUS GAS UNDER CONSTANT DENSITY

A. Equations of equilibrium

We now apply the previous formalism to a homogeneous weakly interacting Bose gas with volume V and particle number N . The interaction we adopt is given by

$$\mathcal{U}(\mathbf{r} - \mathbf{r}') = \frac{4\pi\hbar^2 a}{m} \delta(\mathbf{r} - \mathbf{r}'), \quad (33)$$

where m is the particle mass and a is the s -wave scattering length. The important dimensionless parameter of the system is given by

$$\delta = an^{1/3}, \quad (34)$$

with $n \equiv N/V$, which completely characterizes the properties of $\delta \ll 1$.

The corresponding condensate wave function and the quasiparticle eigenfunctions are the plane waves:

$$\Psi(\mathbf{r}) = \sqrt{n_0}, \quad (35)$$

$$\hat{u}_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k} \cdot \mathbf{r}} \begin{bmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ -v_{\mathbf{k}} & u_{\mathbf{k}} \end{bmatrix}, \quad (36)$$

with $n_0 \equiv N_0/V$ denoting the condensate density. It should be pointed out that the definition of $\hat{u}_{\mathbf{k}}(\mathbf{r})$ above is slightly different from Eq. (25a). Indeed, $\hat{u}_{\mathbf{k}}(\mathbf{r})$ is composed of $\vec{u}_{\mathbf{k}}(\mathbf{r})$ and $-\hat{\tau}_3 \vec{u}_{-\mathbf{k}}^*(\mathbf{r})$ with the common spatial dependence $e^{i\mathbf{k} \cdot \mathbf{r}}$, which is more convenient for the homogeneous case. The coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are chosen real; they clearly have the symmetry: $u_{-\mathbf{k}} = u_{\mathbf{k}}$ and $v_{-\mathbf{k}} = v_{\mathbf{k}}$.

Accordingly, Eq. (13) can be expanded as

$$\hat{\Sigma}(\mathbf{r}, \mathbf{r}') = \frac{1}{V} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \begin{bmatrix} \Sigma & \Delta \\ -\Delta & -\Sigma \end{bmatrix}, \quad (37)$$

where the coefficients Σ and Δ have no \mathbf{k} dependence for the contact interaction. The Hartree-Fock energy Σ is obtained from Eqs. (14a), (17), and (33) as

$$\Sigma = \frac{8\pi\hbar^2 na}{m}. \quad (38)$$

It merely shifts the chemical potential and does not play an important role in the thermodynamics with constant density. Substitution of Eqs. (35) and (37) into Eq. (16) yields the Hugenholtz-Pines relation:

$$\mu_s = \Sigma - \Delta. \quad (39)$$

Hence the excitation spectrum has no energy gap in our mean-field theory.

The quasiparticle eigenstates are obtained by substituting Eqs. (36) and (37) into Eqs. (18) and (24) and diagonalizing the resulting 2×2 matrix in \mathbf{k} space. We thereby arrive at the well-known expressions:³⁰

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}(\epsilon_{\mathbf{k}} + 2\Delta)}, \quad (40a)$$

$$u_{\mathbf{k}} = \sqrt{\frac{\xi_{\mathbf{k}} + E_{\mathbf{k}}}{2E_{\mathbf{k}}}}, \quad v_{\mathbf{k}} = \sqrt{\frac{\xi_{\mathbf{k}} - E_{\mathbf{k}}}{2E_{\mathbf{k}}}}, \quad (40b)$$

with $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$ and $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Delta$. Putting them back into Eqs. (14b) and (17) with Eq. (30), we obtain

$$n = n_0 + A \left(\int_0^\infty \frac{\xi}{E} \frac{\varepsilon^{1/2}}{e^{E/T} - 1} d\varepsilon + \frac{\sqrt{2}}{3} \Delta^{3/2} \right), \quad (41)$$

$$\Delta = \frac{4\pi\hbar^2 a}{m} \left[n_0 + A \left(\int_0^\infty \frac{\Delta}{E} \frac{\varepsilon^{1/2}}{e^{E/T} - 1} d\varepsilon + \Delta \varepsilon_c^{1/2} \right) \right], \quad (42)$$

where $A \equiv m^{3/2}/\sqrt{2\pi^2\hbar^3}$ is a numerical constant, and we have introduced an energy cutoff ε_c in Eq. (42) to remove an ultraviolet divergence inherent in the contact interaction. Equations (41) and (42) forms coupled self-consistent equations for n_0 and Δ , which completely determines the thermodynamic equilibrium at a given temperature.

Once n_0 and Δ are obtained by Eqs. (41) and (42), we can calculate equilibrium thermodynamic properties such as the pressure p_s , the entropy S_s , and the superfluid density ρ_s . Pressure $p_s = -\Omega_{\text{eq}}/V$ is transformed from Eq. (31) into

$$p_s = \frac{\Sigma}{2}n - \frac{\Delta}{2}n_0 + A \int_0^\infty \left(\frac{2\varepsilon\xi}{3E} - \frac{\Delta^2}{2E} \right) \frac{\varepsilon^{1/2}}{e^{E/T} - 1} d\varepsilon - \frac{A}{15\sqrt{2}}\Delta^{5/2}. \quad (43)$$

Equation (32) for S_s now reads

$$\frac{S_s}{N} = \frac{A}{nT} \int_0^\infty \frac{5\xi + 3\Delta}{3E} \frac{\varepsilon^{3/2}}{e^{E/T} - 1} d\varepsilon. \quad (44)$$

The expression of ρ_s is given by³⁰

$$\rho_s = mn \left[1 - \frac{2A}{3nT} \int_0^\infty \frac{\varepsilon^{3/2} e^{E/T}}{(e^{E/T} - 1)^2} d\varepsilon \right]. \quad (45)$$

The constant A in Eqs. (41)-(45) under constant density may be written alternatively in terms of the transition temperature of the ideal Bose gas $T_0 = (2\pi\hbar^2/m)[n/\zeta(\frac{3}{2})]^{2/3}$ as

$$A = \frac{2n}{\sqrt{\pi}\zeta(\frac{3}{2})T_0^{3/2}}, \quad (46)$$

with $\zeta(\frac{3}{2}) = 2.61$ denoting the Riemann ζ function. It is convenient to choose T_0 as the unit of energy. Then Eq. (42), for example, reads

$$\left[1 - \frac{4\varepsilon_c^{1/2}\delta}{\sqrt{\pi}\zeta(\frac{3}{2})^{1/3}} \right] \Delta = 2\zeta(\frac{3}{2})^{2/3}\delta \left[\frac{n_0}{n} + \frac{2}{\sqrt{\pi}\zeta(\frac{3}{2})} \int_0^\infty \frac{\Delta}{E} \frac{\varepsilon^{1/2}}{e^{E/T} - 1} d\varepsilon \right]. \quad (47)$$

We choose the cutoff ε_c so that $1 \ll \varepsilon_c \ll 0.3\delta^{-2}$ is satisfied and neglect the cutoff-dependent term in the following. This does not affect the results qualitatively, and even quantitatively to the leading order in δ .

Numerical calculations of Eqs. (41)-(45) can be performed easily to clarify temperature dependences of the basic thermodynamic quantities in the condensed phase. A change of variable $\varepsilon = 2\Delta \sinh^2 t$ is found to improve convergence of the integrations including $e^{E/T}$. The corresponding equations for the normal state are obtained from Eqs. (41), (43), and (44) by setting $\Delta = n_0 = 0$ and

$E = \xi = \varepsilon + \Sigma - \mu_n$, which yield μ_n , p_n , and S_n as a function of T . The transition temperature T_c is then determined by the thermodynamic condition $F_s(T_c, V, N) = F_n(T_c, V, N)$ appropriate under constant volume. The specific heat C may be calculated from the results on S by numerical differentiations.

B. Properties near T_c

We now investigate the properties near T_c ($\sim T_0 = 1$) in more detail. To this end, we make use of the following asymptotic expansions for the integrals in Eqs. (41)-(43), respectively:

$$\frac{2}{\sqrt{\pi}\zeta(\frac{3}{2})} \int_0^\infty \frac{\xi}{E} \frac{\varepsilon^{1/2}}{e^{E/T} - 1} d\varepsilon = T^{3/2}(1 - b_1 x^{1/2}), \quad (48a)$$

$$\frac{2}{\sqrt{\pi}\zeta(\frac{3}{2})} \int_0^\infty \frac{\Delta}{E} \frac{\varepsilon^{1/2}}{e^{E/T} - 1} d\varepsilon = T^{3/2}b_1 x^{1/2}, \quad (48b)$$

$$\frac{2}{\sqrt{\pi}\zeta(\frac{5}{2})} \int_0^\infty \left(\frac{2\varepsilon\xi}{3E} - \frac{\Delta^2}{2E} \right) \frac{\varepsilon^{1/2}}{e^{E/T} - 1} d\varepsilon = T^{5/2}(1 - b_1''x + b_2''x^{3/2}), \quad (48c)$$

with $x \equiv \Delta/T$, $b_1 \equiv \sqrt{2\pi}/\zeta(\frac{3}{2}) = 0.960$, $b_1'' \equiv \zeta(\frac{3}{2})/\zeta(\frac{5}{2}) = 1.95$, and $b_2'' \equiv 5\sqrt{2\pi}/6\zeta(\frac{5}{2}) = 1.56$. Each expression of Eq. (48) has been obtained as follows: (i) Expand the integrand in terms of Δ up to the order where the integral converges to obtain the leading terms analytic in x . (ii) Subtract the leading contribution from the original integral to express the residual term as an integral. (iii) Estimate the higher-order integral by expanding the exponentials in the denominators up to the first order. For example, analytic terms are absent in Eq. (48b), and the integral has been estimated by approximating $e^{E/T} - 1 \approx E/T$ in the denominator. Those residual integrals generally yield terms non-analytic in x . This non-analyticity in the expansion near T_c is inherent in Bose systems stemming from the divergence of the Bose distribution function at zero energy. This is in marked contrast to the weak-coupling theory of superconductivity where the gap equation near T_c is analytic in $x^2 \equiv (\Delta/T)^2$ to make the Landau-Ginzburg expansion possible.⁵⁷ Thus, unlike the Ginzburg-Landau equations for superconductors,⁵⁸ the Ginzburg-Pitaevskii equation⁵⁹ for the condensed Bose systems cannot be justified microscopically. It is this non-analyticity which turns the mean-field transition into first order and also brings various anomalies in the thermodynamic properties near T_c which cannot be described by the Landau theory of second-order transition.⁶⁰

Substituting Eqs. (48a) and (48b) into Eqs. (41) and (42), respectively, we obtain

$$\frac{n_0}{n} = 1 - T^{3/2}(1 - b_1 y + b_2 y^2), \quad (49a)$$

$$\frac{n_0}{n} = \frac{1 + b'_2 c T^{1/2} \delta}{c \delta} T y \left(y - \frac{b_1 c T^{1/2} \delta}{1 + b'_2 c T^{1/2} \delta} \right), \quad (49b)$$

with $y \equiv x^{1/2} = (\Delta/T)^{1/2}$, $b_2 = 0.559$, $b'_2 = 1.12$, and $c = 2\zeta(\frac{3}{2})^{2/3} = 3.79$. Here we have used the results of Eqs. (48a) and (48b) including higher-order terms $b_2 x$ and $-b'_2 x$, respectively, with b_2 and b'_2 estimated numerically.⁶¹ Let us subtract Eq. (49b) from Eq. (49a). Solving the resulting equation, we obtain y as a function of T as

$$y(T) = \frac{b_1 c T^{1/2} \delta}{1 + (b_2 + b'_2) c T^{1/2} \delta} \left\{ 1 + \left[1 - \frac{T^{-\frac{1}{2}} - T^{-2}}{b_1^2 c \delta} \times [1 + (b_2 + b'_2) c T^{1/2} \delta] \right]^{1/2} \right\}. \quad (50)$$

The transition temperature T_c may be estimated by setting $n_0 = 0$ in Eq. (49b), which yields

$$y(T_c) - \frac{b_1 c T_c^{1/2} \delta}{1 + b'_2 c T_c^{1/2} \delta} = 0. \quad (51)$$

Equation (51) with Eq. (50) can be solved by expanding T_c in powers of δ as

$$T_c = 1 + \frac{8\pi}{3\zeta(\frac{3}{2})^{4/3}} \delta + \frac{8\pi}{3\zeta(\frac{3}{2})^{4/3}} \left[\frac{14\pi}{3\zeta(\frac{3}{2})^{4/3}} - (b_2 + b'_2) c \right] \delta^2 \\ = 1 + 2.33\delta + \dots \quad (52)$$

Thus, T_c initially increases linearly with δ . The numerical coefficient 2.33 agrees with the analytic result by Baym *et al.*³⁴ as well as the numerical one by Holzmann and Krauth.³³ It is worth pointing out that this expression makes the coefficients of δ^0 and δ in the large square bracket of Eq. (50) vanish at T_c . Substituting Eq. (52) into Eq. (51) and noting $y \equiv (\Delta/T)^{1/2}$, we obtain

$$\Delta(T_c) = \frac{8\pi}{\zeta(\frac{3}{2})^{2/3}} \delta^2 = 13.3\delta^2, \quad (53)$$

to the leading order in δ .

A comment is necessary on Eq. (52) at this stage. The expression (52) has been obtained as the highest temperature of the non-trivial solutions to Eq. (49). However, the corresponding superfluid transition is first-order. It hence follows that, under the present conditions of fixed V and N , the transition temperature should have been determined alternatively by the requirement that the free energy $F(T, V, N)$ be equal between the normal and superfluid phases. It will be shown below Eq. (65), however, that Eq. (52) indeed satisfies the requirement up to the order δ^2 .

We next consider the region below T_c and expand $y(T) - y(T_c)$ in powers of $1 - T/T_c$. As noted below Eq. (52), the leading term at T_c in the large square bracket of Eq. (50) is proportional to δ^2 . The proportionality

constant is found to be $(b_2 c)^2$ from the equation of order δ^3 in the expansion of Eq. (52). Due to this smallness of the constant term at $T = T_c$, the temperature-dependent contribution $\propto (1 - T/T_c)$ in the square bracket may not be placed outside. Indeed, we obtain

$$y(T) - y(T_c) \\ = -b_1 b_2 c^2 \delta^2 + \left[(b_1 b_2 c^2 \delta^2)^2 + \frac{3}{2} c \delta (1 - T/T_c) \right]^{1/2} \\ \approx \begin{cases} 0.369 \delta^{-1} (1 - T/T_c) & : 1 - T/T_c \ll 10.5 \delta^3 \\ \sqrt{3} \zeta(\frac{3}{2})^{1/3} \delta^{1/2} (1 - T/T_c)^{1/2} & : 1 - T/T_c \gg 10.5 \delta^3 \end{cases}. \quad (54)$$

Noting $y = (\Delta/T)^{1/2}$ and Eq. (53), we may approximate Δ just below T_c as

$$\Delta(T) - \Delta(T_c) \\ = \begin{cases} 2.69 (1 - T/T_c) & : 1 - T/T_c \ll 10.5 \delta^3 \\ \sqrt{96\pi} \delta^{3/2} (1 - T/T_c)^{1/2} & : 1 - T/T_c \gg 10.5 \delta^3 \end{cases}. \quad (55)$$

Let us substitute Eqs. (53) and (54) into Eq. (49b). We then find that $n_0(T)$ grows as

$$\frac{n_0}{n} = \begin{cases} 0.354 \delta^{-1} (1 - T/T_c) & : 1 - T/T_c \ll 10.5 \delta^3 \\ \frac{\sqrt{6\pi}}{\zeta(\frac{3}{2})^{2/3}} \delta^{1/2} (1 - T/T_c)^{1/2} & : 1 - T/T_c \gg 10.5 \delta^3 \end{cases}. \quad (56)$$

Equations (52), (53), (55), and (56) are the main results obtained from Eq. (49).

We turn our attention to other thermodynamic quantities. The chemical potential below T_c satisfies the Hugenholtz-Pines relation $\mu_s(T) = \Sigma - \Delta(T)$ and directly reflects the singularity of $\Delta(T)$ near T_c . On the other hand, $\mu_n(T)$ in the normal state of $T \gtrsim 1$ obeys

$$\mu_n(T) = \Sigma - \frac{\zeta(\frac{3}{2})^2}{4\pi} (T^{3/2} - 1)^2. \quad (57)$$

This can be shown from $N = \sum_{\mathbf{k}} [e^{(\epsilon_{\mathbf{k}} + \Sigma - \mu_n)/T} - 1]^{-1}$ with the procedure of deriving the expansions of Eq. (48). Using Eqs. (52) and (53), we obtain the discontinuity $\Delta\mu(T_c) \equiv \mu_s(T_c) - \mu_n(T_c)$ as

$$\Delta\mu(T_c) = -\frac{4\pi}{\zeta(\frac{3}{2})^{2/3}} \delta^2 = -6.63\delta^2. \quad (58)$$

Next, with the procedure of deriving Eq. (48), the entropy just below T_c is calculated from Eq. (44) as

$$\frac{S_s}{N} = \frac{5\zeta(\frac{5}{2})}{2\zeta(\frac{3}{2})} T^{3/2} - \frac{3}{2} T^{1/2} \Delta. \quad (59)$$

The corresponding normal-state expression for $T \gtrsim 1$ is given by

$$\frac{S_n}{N} = \frac{5\zeta(\frac{5}{2})}{2\zeta(\frac{3}{2})} T^{3/2} - \frac{3\zeta(\frac{3}{2})^2}{8\pi} (T^{3/2} - 1)^2. \quad (60)$$

Hence the discontinuity $\Delta S(T_c) \equiv S_s(T_c) - S_n(T_c)$ is found by using Eqs. (52) and (53) as

$$\Delta S(T_c) = -\frac{6\pi}{\zeta(\frac{3}{2})^{2/3}}\delta^2 = -9.94\delta^2. \quad (61)$$

It follows from Eqs. (55) and (59) that the specific heat $C_s = T(\partial S_s/\partial T)$ just below T_c is given to the leading order by

$$\begin{aligned} \frac{C_s}{N} &= \frac{15\zeta(\frac{5}{2})}{4\zeta(\frac{3}{2})}T^{3/2} - \frac{3}{2}T^{3/2}\frac{d\Delta}{dT} \\ &= \frac{C_n}{N} + \begin{cases} 4.04 & : 1 - T/T_c \ll 10.5\delta^3 \\ \frac{3\sqrt{6\pi}\delta^{3/2}}{(1 - T/T_c)^{1/2}} & : 1 - T/T_c \gg 10.5\delta^3 \end{cases}. \end{aligned} \quad (62)$$

It displays a divergent behavior $C_s/N \sim 13.0\delta^{3/2}(1 - T/T_c)^{-1/2}$ for $10.5\delta^3 \ll 1 - T/T_c \ll 1$.

Substituting Eq. (48c) into Eq. (43), p_s just below T_c is obtained as

$$\frac{p_s}{n} = \frac{\Sigma}{2} - \frac{\Delta}{2} \frac{n_0}{n} + \frac{\zeta(\frac{5}{2})}{\zeta(\frac{3}{2})}T^{5/2} - T^{3/2}\Delta. \quad (63)$$

The normal-state pressure of $T \gtrsim 1$ can be calculated similarly to be

$$\frac{p_n}{n} = \frac{\Sigma}{2} + \frac{\zeta(\frac{5}{2})}{\zeta(\frac{3}{2})}T^{5/2} - \frac{\zeta(\frac{3}{2})^2}{4\pi}(T^{3/2} - 1)^2. \quad (64)$$

Hence the discontinuity $\Delta p(T_c) \equiv p_s(T_c) - p_n(T_c)$ is obtained as

$$\frac{\Delta p(T_c)}{n} = -\frac{4\pi}{\zeta(\frac{3}{2})^{2/3}}\delta^2 = -6.63\delta^2. \quad (65)$$

It follows from Eqs. (58) and (65) as well as $F(T, V, N) = -pV + \mu N$ that $F_s(T_c, V, N) = F_n(T_c, V, N)$ is satisfied for the expression (52) up to the order δ^2 . Thus, Eq. (52) is indeed a correct expression of T_c of order δ .

We finally consider the superfluid density near T_c . With the procedure of deriving Eq. (48), Eq. (45) is transformed into

$$\frac{\rho_s}{mn} = 1 - T^{3/2} + \frac{4\sqrt{2\pi}T\Delta^{1/2}}{3\zeta(\frac{3}{2})}. \quad (66)$$

Substituting Eqs. (52) and (53) into Eq. (66), we obtain

$$\frac{\Delta\rho_s(T_c)}{mn} = \frac{4\pi}{3\zeta(\frac{3}{2})^{4/3}}\delta = 1.16\delta. \quad (67)$$

C. Properties at $T = 0$

Physical properties at $T = 0$ are easily found from Eqs. (39) and (41)-(45) by dropping terms with the Bose

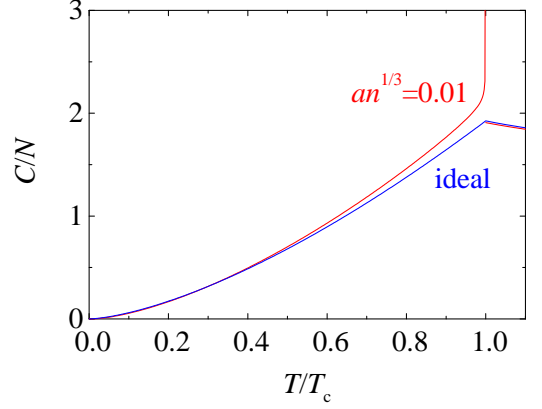


FIG. 2: Specific heat C/N as a function of T/T_c for $an^{1/3} = 0.01$ shown in comparison with the ideal gas result.

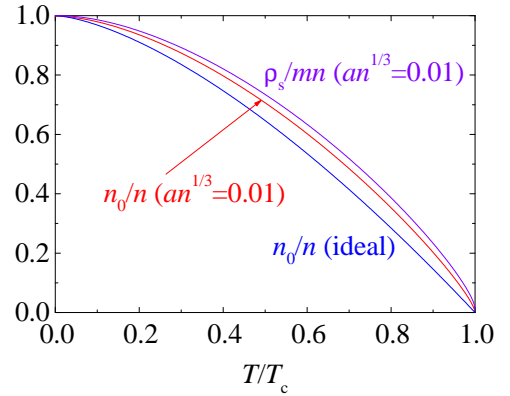


FIG. 3: Normalized condensate density n_0/n and superfluid density ρ_s/nm as a function of T/T_c for $an^{1/3} = 0.01$. The ideal gas result ($n_0/n = \rho_s/nm$) is also plotted for comparison.

distribution function. The leading-order expressions are summarized as follows:

$$\frac{n_0(0)}{n} = 1 - \frac{8}{3\sqrt{\pi}}\delta^{3/2} = 1 - 1.50\delta^{3/2}, \quad (68a)$$

$$\mu_s(0) = \Delta(0) = 2\frac{p_s(0)}{n} = 2\zeta(\frac{3}{2})^{2/3}\delta = 3.79\delta. \quad (68b)$$

D. Numerical Results

Figure 2 displays the specific heat C/N as a function of the renormalized temperature T/T_c for $an^{1/3} = 0.01$. The ideal-gas result ($a = 0; T_c = T_0$) is also plotted for comparison. The curve for $an^{1/3} = 0.01$ is proportional to T^3 at very low temperatures due to $E_{\mathbf{k}} \propto k$ for $k \rightarrow 0$. As the temperature is increased, the curve starts to deviate

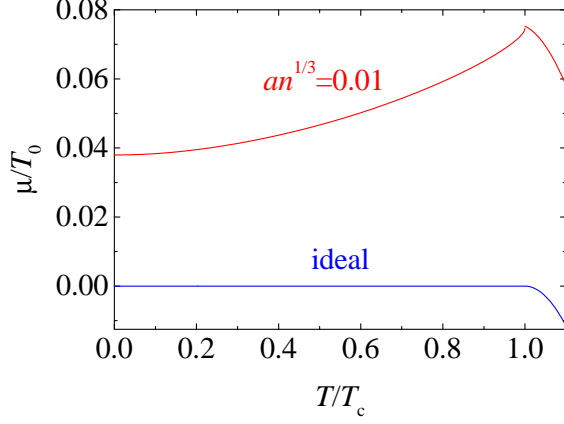


FIG. 4: Temperature dependence of the chemical potential μ for $an^{1/3} = 0.01$ shown in comparison with the ideal gas result.

upward from the ideal-gas result to show the limiting behavior (62) for $T \lesssim T_c$.

Figure 3 plots n_0/n and ρ_s/nm as a function of T/T_c for $an^{1/3} = 0.01$ and 0. We observe that the finite interaction causes an enhancement of n_0/n and ρ_s/nm over the ideal-gas value at all temperatures. The enhancement is larger for ρ_s/nm than n_0/n . The quantity n_0/n obeys Eq. (56) near T_c and develops continuously from 0 even with a finite interaction, whereas ρ_s/nm starts from a positive value at T_c as Eq. (67).

Figure 4 shows the chemical potential as a function of T/T_c for $an^{1/3} = 0.01$ and 0. With a finite interaction, the chemical potential displays a characteristic peak at T_c with a discontinuity, as shown explicitly by Eq. (58). It eventually approaches the value of Eq. (68b) as the temperature is lowered.

E. The HFB and Shohno theories

We now compare the above predictions of the conserving gapless mean-field theory with those of the HFB^{14,21,29,45} and Shohno^{22,29} theories. Although extensive theoretical studies have been carried out based on the latter theories, their predictions on the thermodynamic quantities seem not to have been clarified completely, especially near T_c . We hence study them in detail with a special focus on the region $T \lesssim T_c$. This will also help us to understand common features in the mean-field theories of the homogenous weakly interacting Bose gas. The transition temperature will be determined below in the same way as Eq. (52); the two comments below Eqs. (53) and (65) also apply to the present cases.

The equations to determine the equilibrium in the HFB theory are formally obtained from Eqs. (41) and (42) by a couple of modifications: (i) a sign change for the second term in the square bracket of Eq. (42); (ii) the expressions

of $\xi_{\mathbf{k}}$ and $E_{\mathbf{k}}$. Indeed, they are given by

$$n = n_0 + \frac{1}{V} \sum_{\mathbf{k}} \left(\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \frac{1}{e^{E_{\mathbf{k}}/T} - 1} + \frac{\xi_{\mathbf{k}} - E_{\mathbf{k}}}{2E_{\mathbf{k}}} \right), \quad (69a)$$

$$\Delta = \frac{4\pi\hbar^2 a}{m} n_0 - \Gamma, \quad (69b)$$

where Γ , $\xi_{\mathbf{k}}$, and $E_{\mathbf{k}}$ are defined by

$$\Gamma \equiv \frac{4\pi\hbar^2 a}{mV} \sum_{\mathbf{k}} \left(\frac{\Delta}{E_{\mathbf{k}}} \frac{1}{e^{E_{\mathbf{k}}/T} - 1} + \frac{\Delta}{2E_{\mathbf{k}}} \right), \quad (70)$$

$$\xi_{\mathbf{k}} \equiv \varepsilon_{\mathbf{k}} + \Delta + 2\Gamma, \quad E_{\mathbf{k}} \equiv \sqrt{(\varepsilon_{\mathbf{k}} + 2\Gamma)(\varepsilon_{\mathbf{k}} + 2\Delta + 2\Gamma)}, \quad (71)$$

with $\varepsilon_{\mathbf{k}} \equiv \hbar^2 k^2 / 2m$. The Shohno theory is obtained from Eqs. (69) and (71) by setting $\Gamma = 0$.

Near $T \sim T_0 = 1$ where Δ and Γ are much smaller than T_0 , Eq. (69) is approximated to the leading order by

$$\frac{n_0}{n} = 1 - T^{3/2} [1 - b_1 (\sqrt{\Gamma + \Delta} + \sqrt{\Gamma})], \quad (72a)$$

$$\Delta = c\delta \left[\frac{n_0}{n} - b_1 (\sqrt{\Gamma + \Delta} - \sqrt{\Gamma}) \right], \quad (72b)$$

with $b_1 \equiv \sqrt{2\pi}/\zeta(\frac{3}{2})$ and $c = 2\zeta(\frac{3}{2})^{2/3}$. These equations correspond to Eq. (49) and have been obtained with the procedure of deriving the expansions of Eq. (48). Note that Eq. (72) is also non-analytic in Γ and $\Gamma + \Delta$. Using $\Delta = c\delta(n_0/n - \Gamma)$ from Eq. (69b), we next rewrite Eq. (72b) in terms of Γ and n_0/n . We also introduce the dimensionless variables r , s , and t through $\sqrt{n_0/n} = b_1 \sqrt{c\delta} r$, $\sqrt{\Gamma} = b_1 c\delta s$, and $T = 1 + b_1^2 c\delta t$. Retaining terms of order δ , Eq. (72) is transformed into

$$r^2 - r + \frac{3}{2}t = s, \quad s = \frac{-1 + \sqrt{1 + 4r}}{2}. \quad (73)$$

Equation (73) yields

$$f(r, t) \equiv r^4 - 2r^3 + (2+3t)r^2 - (2+3t)r + \frac{3}{4}t(2+3t) = 0. \quad (74)$$

It has a couple of solutions $r_1, r_2 > 0$ for $t \approx 0$ but no real solution for a large-enough t . Thus, the transition temperature corresponds to the point where $f = 0$ and $\partial f / \partial r = 0$, which yields the critical values of $t = 11/24$ and $r = 3/4$. Thus, the transition temperature of the HFB theory for $\delta \rightarrow 0$ is given by $T_c^{\text{HFB}} = 1 + \Delta T_c^{\text{HFB}}$ with

$$\Delta T_c^{\text{HFB}} = \frac{11\pi}{6\zeta(\frac{3}{2})^{4/3}} \delta = 1.60\delta. \quad (75a)$$

The transition is clearly first order. The discontinuities of various thermodynamic quantities at T_c^{HFB} can be obtained with the procedure of Sec. III B as

$$\frac{n_0^{\text{HFB}}(T_c)}{n} = \frac{9\pi}{4\zeta(\frac{3}{2})^{4/3}} \delta = 1.96\delta, \quad (75b)$$

$$\Delta^{\text{HFB}}(T_c) = \frac{5\pi}{2\zeta(\frac{3}{2})^{2/3}}\delta^2 = 4.14\delta^2, \quad (75c)$$

$$\frac{\rho_s^{\text{HFB}}(T_c)}{mn} = \frac{139\pi}{60\zeta(\frac{3}{2})^{4/3}}\delta = 2.02\delta. \quad (75d)$$

Note that even n_0/n is discontinuous at T_c in the HFB theory.

The same analysis can be performed for the Shohno theory. We thereby obtain

$$\Delta T_c^{\text{Shohno}} = \frac{2\pi}{3\zeta(\frac{3}{2})^{4/3}}\delta = 0.582\delta, \quad (76a)$$

$$\frac{n_0^{\text{Shohno}}(T_c)}{n} = \frac{\pi}{\zeta(\frac{3}{2})^{4/3}}\delta = 0.873\delta, \quad (76b)$$

$$\Delta^{\text{Shohno}}(T_c) = \frac{2\pi}{\zeta(\frac{3}{2})^{2/3}}\delta^2 = 3.31\delta^2, \quad (76c)$$

$$\frac{\rho_s^{\text{Shohno}}(T_c)}{mn} = \frac{5\pi}{3\zeta(\frac{3}{2})^{4/3}}\delta = 1.46\delta. \quad (76d)$$

Thus, even the Shohno theory predicts an enhancement of T_c over the ideal-gas value T_0 .

As for the overall temperature dependences of various thermodynamic quantities, the HFB and Shohno theories both yield results qualitatively similar to those of the previous mean-field theory except the discontinuity of n_0 at T_c . For example, the specific heat of the HFB and Shohno theories also display the divergent behavior of $(T_c - T)^{-1/2}$ just below T_c . Due to a finite Γ , the HFB theory generally predicts larger deviations from the ideal-gas results than the Shohno theory.

IV. HOMOGENEOUS GAS UNDER CONSTANT DENSITY

We finally study the homogeneous weakly interacting Bose gas under the complementary condition of constant pressure. Despite its fundamental importance as a subject of quantum statistical mechanics, the system seems to have been investigated only by Reatto and Straley²⁹ based on the HFB and Shohno theories.^{29,45} Moreover, their main interest was on superfluid ⁴He so that the properties in the weak-coupling region remain essentially unexplored.

Let us introduce a dimensionless parameter δ_p by

$$\delta_p \equiv a \left(\frac{mp}{2\pi\hbar^2} \right)^{1/5}, \quad (77)$$

which completely characterizes the weak-coupling region of $\delta_p \ll 1$. The thermodynamic equilibrium of the condensed phase is determined by Eqs. (41)-(43). They yield the density n , the condensate density n_0 , and the pair potential Δ as a function of p and T . The prefactor A in Eqs. (41)-(43) may be rewritten conveniently as

$$A = \frac{2n_c}{\sqrt{\pi}\zeta(\frac{3}{2})T_0^{3/2}} = \frac{2p}{\sqrt{\pi}\zeta(\frac{5}{2})T_0^{5/2}}, \quad (78)$$

where n_c and T_0 are the critical density and the transition temperature of the ideal Bose gas, respectively. They are given in terms of p as $n_c = [mp/2\pi\hbar^2\zeta(\frac{5}{2})]^{3/5}\zeta(\frac{3}{2})$ and $T_0 = (2\pi\hbar^2/m)^{3/5}[p/\zeta(\frac{5}{2})]^{2/5}$. The equations for the normal state are obtained from Eqs. (41), (43), and (44) by setting $\Delta = n_0 = 0$ and $E = \xi = \varepsilon + \Sigma_n - \mu_n$; they yield n , μ_n , and S_n as a function of p and T . The transition temperature T_c is then determined by the thermodynamic condition $\mu_s(T_c, p) = \mu_n(T_c, p)$ appropriate under constant pressure. The specific heat per particle C_p may be calculated from the results on S by numerical differentiations. In the following, we will adopt the units in which $n_c = T_0 = 1$ and neglect the cutoff-dependent term in Eq. (42) as was done in the case of constant density.

To investigate the properties near T_c (~ 1) in more detail, we make use of the asymptotic expansions of Eq. (48). Equations (41) and (42) with Eq. (48) enable us to express n_0 and n in terms of T and Δ as $n_0 = \Delta/c'\delta_p - b_1T\Delta^{1/2}$ and $n = T^{3/2} + \Delta/c'\delta_p - 2b_1T\Delta^{1/2}$ with $c' \equiv 2\zeta(\frac{3}{2})/\zeta(\frac{5}{2})^{1/5} = 4.93$. Substituting them into it, Eq. (43) becomes a nonlinear equation for Δ as

$$\begin{aligned} & \frac{b_1''}{2c'\delta_p}\Delta^2 - \left(\frac{7b_1b_1''}{2} - b_2'' \right) T\Delta^{3/2} \\ & + \left(b_1''T^{3/2} + 4b_1^2b_1''c'T^2\delta_p \right) \Delta - 4b_1b_1''c'T^{5/2}\delta_p\Delta^{1/2} \\ & + T^{5/2} + b_1''c'T^3\delta_p - 1 = 0. \end{aligned} \quad (79)$$

Thus, the equation is non-analytic in Δ and completely different from the one in the Landau theory of second-order transition.⁶⁰ It is convenient to rewrite T in Eq. (79) as $T = 1 - \frac{2}{5}b_1''c'\delta_p + t\delta_p^2 = 1 - 3.84\delta_p + t\delta_p^2$, where t is a parameter appropriate to describe the region $T \sim 1$. Then Eq. (79) can be solved analytically by expanding Δ as $\Delta = \Delta_2(t)\delta_p^2 + \Delta_3(t)\delta_p^3 + \dots$. The expression for $\Delta_2(t)$ is obtained as

$$\Delta_2(t) = \left[2b_1c' + \sqrt{(2b_1c')^2 + \frac{9b_1''c'^2}{10} - \frac{5}{2b_1''}t} \right]^2. \quad (80a)$$

It hence follows that a superfluid solution exists for $t \leq t_s \equiv (2b_1''/5)[(2b_1c')^2 + 9b_1''c'^2/10] = 103$. The quantity $\Delta_3(t)$ may be expressed in terms of t and $\Delta_2(t)$. A similar consideration for the normal state leads to a nonlinear equation for $\Sigma - \mu$. Expanding $\Sigma - \mu = \Sigma_2(t)\delta_p^2 + \Sigma_3(t)\delta_p^3 + \dots$, $\Sigma_2(t)$ is found to satisfy

$$\sqrt{\Sigma_2(t)} = -\sqrt{2}b_1c' + \sqrt{2(b_1c')^2 - \frac{9b_1''c'^2}{10} + \frac{5}{2b_1''}t}. \quad (80b)$$

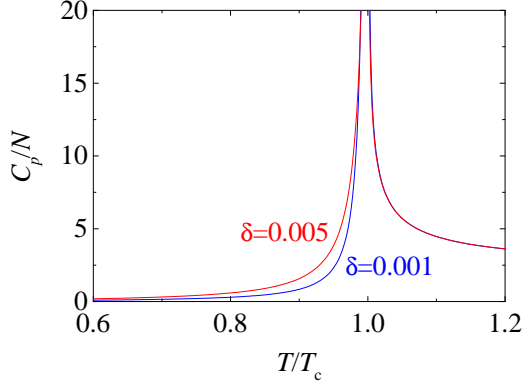


FIG. 5: Specific heat C_p as a function of T/T_c for $\delta_p = 0.001$ and 0.005.

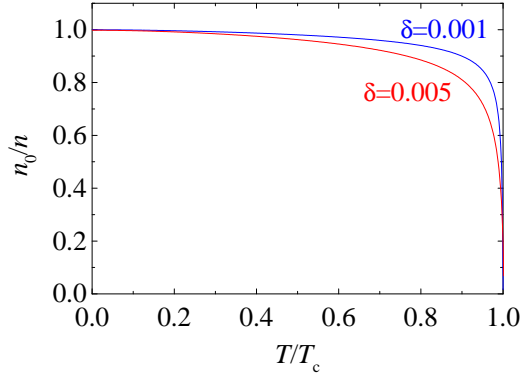


FIG. 6: Normalized condensate density n_0/n as a function of T/T_c for $\delta_p = 0.001$ and 0.005.

It has a real solution Σ_2 for $t \geq t_n \equiv 18(b_1''c')^2/50 = 33.1$.

From $t_s > t_n$, we realize that the superfluid transition is first order with a metastable region extending over $t_n \leq t \leq t_s$. The transition temperature T_c can also be expressed as

$$T_c = 1 - 3.84\delta_p + t_c\delta_p^2. \quad (81)$$

Thus, T_c becomes smaller than $T_0 = 1$ to the leading order in δ_p . This behavior is opposite to the case of constant volume where T_c increases as a function of the dimensionless parameter $an^{1/3}$.⁴² Indeed, the effect of the weak repulsive interaction is completely different between the volume-fixed and pressure-fixed cases. In the former case, a finite interaction suppresses the density fluctuation so that it works favorably for the phase coherence over the system, thereby leading to an enhancement of T_c . In the latter case, on the other hand, the interaction lowers the particle density to decrease T_c . The value of the prefactor 3.84 is almost certainly correct, in contrast to the volume-fixed case where it seems still controversial.^{42,43}

We turn our attention to t_c of Eq. (81) which includes all the higher-order contributions. It is found that t_c

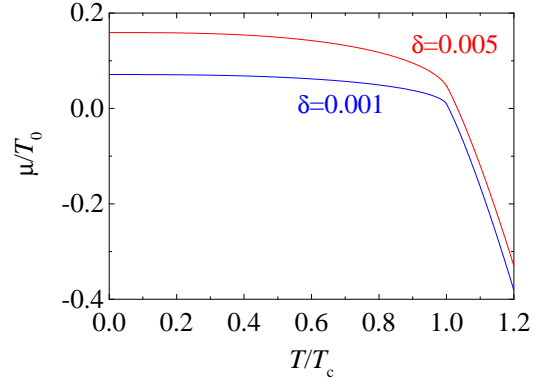


FIG. 7: Chemical potential as a function of T/T_c for $\delta_p = 0.001$ and 0.005.

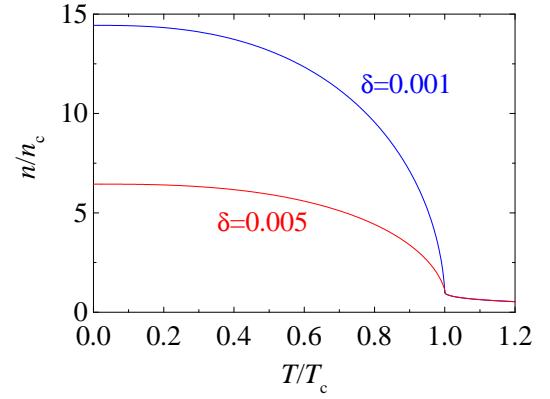


FIG. 8: Normalized particle density n/n_c as a function of T/T_c for $\delta_p = 0.001$ and 0.005.

has a rather large δ_p dependence, due partly to the large values of the numerical constants appearing in the equations, e.g., $t_s = 103$. It decreases from $t_c(\delta_p \rightarrow 0) = t_s = 103$ down to 98.6, 96.9, and 95.7 at $\delta_p = 5.0 \times 10^{-4}$, 1.0×10^{-3} , and 1.5×10^{-3} , respectively. The contributions from Δ_3 and Σ_3 are essential to produce the results, which agree excellently with the exact numerical results of using Eqs. (41)-(43) for $T \sim 1$. Discontinuities in the thermodynamic quantities at T_c are found to be all of the order of δ_p^2 in accordance with the tiny metastable region.

Let us move onto the overall temperature dependences of various thermodynamic quantities. Figure 5 plots specific heat C_p over $0.6T_c \leq T \leq 1.2T_c$ for $\delta_p = 0.001$ and 0.005. A remarkable enhancement of C_p near T_c is clearly seen. Indeed, the curves show a divergent behavior $\propto |T - T_c|^{-1/2}$ on both sides near T_c . It is completely different from the discontinuous behavior predicted by the Landau theory of second-order transition and caused by the non-analytic nature of the order-parameter expansion near T_c . The sharp heat absorption/emission near T_c may be realized in terms of the proximity to the ideal Bose gas under constant pressure which sud-

denly falls into the ground state of volume zero below T_0 . The weak repulsive interaction weakens the singularity of the ideal Bose gas at $T = T_0$ over a finite range close to T_c . This sharp absorption/emission of heat near T_c in the present system is in qualitative agreement with the observation on ^4He .⁴⁹ Figure 6 shows the normalized condensate density n_0/n as a function of temperature, where a steep change just below T_c can also be seen clearly. Although not plotted here, the normalized superfluid density $\rho_s(T)/mn(T)$ is almost indistinguishable in the present scale from $n_0(T)/n(T)$ for both $\delta_p = 0.001$ and 0.005 . Figure 7 displays temperature dependence of the chemical potential μ . The curves flatten out rapidly below T_c reflecting proximity to the ground state. Finally, Fig. 8 plots the particle density n as a function of temperature for $\delta_p = 0.001$ and 0.005 . Since the superfluid component contributes less to the pressure than the normal component in the weak-coupling region, a constant pressure can only be sustained at lower temperatures by increasing the particle density. Thus, $n(T)$ increases monotonically as T is lowered from T_c . The leading-order expression of $n(0)$ is given by $n(0)/n_c = [\zeta(\frac{5}{2})^{3/5}/\zeta(\frac{5}{2})]\delta_p^{-1/2} = 0.457\delta_p^{-1/2}$, implying a smaller enhancement of $n(0)$ for a stronger interaction. In this respect, it is worth pointing out that $n(T)$ of superfluid ^4He displays a maximum at T_c .⁴⁹ Whether $n(0)/n(T_c)$ may be reduced beyond 1 or not in the strong-coupling region remains a challenging problem to be clarified theoretically.

V. SUMMARY

We have constructed a mean-field theory for Bose-Einstein condensates. The basic equations to determine the equilibrium are given by Eqs. (14)-(18), (24), and (30). They can be applicable to general non-uniform systems such as the trapped atomic gases with or without vortices. The present theory has a manifest advantage over the HFB and Shohnho theories that it simultaneously satisfies the Hugenholtz-Pines theorem and various conservation laws. It will be useful in clarifying both equilibrium and dynamical properties of condensed Bose gases over the whole temperature range. The conserving gapless theory is expected to provide at least a qualitative description of weakly interacting BEC. Especially, it will shed a new light on the temperature dependences of the collective modes in BEC. It may also form a starting point for a unified description of BEC over the whole interaction strengths from the trapped weakly interacting atomic gases to superfluid ^4He .

The theory is then applied to a homogeneous weakly interacting Bose gas with s -wave scattering length a under constant density n in Sec. III and under constant pressure p in Sec. IV. The order-parameter expansion near T_c is found not of the Landau-Ginzburg type but non-analytic by nature due to the divergence of the Bose distribution function at zero energy, as shown explicitly

in Sec. IIIB. This non-analyticity makes the superfluid transition first-order and also brings unique temperature dependences of various thermodynamic quantities near T_c which are quite different from those of the Landau theory of second-order transition. The transition temperature T_c under constant n is found to increase from the ideal Bose gas value T_0 as $T_c/T_0 = 1 + 2.33an^{1/3}T_0$, whereas it decreases under constant pressure as $T_c/T_0 = 1 - 3.84a(mp/2\pi\hbar^2)^{1/5}$. We have also clarified overall temperature dependences of basic thermodynamic quantities in Secs. IIID and IV. These predictions are then compared with those of the HFB^{14,21,29,45} and Shohnho^{22,29} theories in Sec. IIIE. Those theories also predict a first-order transition and an enhancement of T_c .

We finally comment on the first-order superfluid transition of the present mean-field theory. As mentioned above, it is a feature inherent in the mean-field theories of BEC stemming from the non-analyticity of the Bose distribution function at zero energy. However, it is in contradiction to the observation of superfluid ^4He where the transition is continuous. It has been pointed out by Reatto and Straley²⁹ that the mean-field transition would be continuous if the change of the single-particle dispersion at T_c were from k^ϵ to $k^{\epsilon/2}$ with $\epsilon < \frac{3}{2}$ (k : wave number). The behavior k^ϵ with $\epsilon < \frac{3}{2}$ above T_c may only be possible by including correlations and/or fluctuations. Thus, we encounter the question of whether the correlations and/or fluctuations are essential even in the limit $a \rightarrow 0$ to transform the nature of the superfluid transition. If not so, the transition is expected to change its character from first-order into continuous at an intermediate value of a . Thus, the predictions of the mean-field theory raise the questions on: (i) the relative importance of the single-particle and collective excitations in BEC as a function of the interaction strength; (ii) the role of the single-particle excitations in superfluid ^4He above and below T_c . It is worth reminding that the transition of the ideal Bose gas under constant pressure is strongly first-order. Hence it may not be so unreasonable to expect that the first-order transition persists into the region of a finite interaction.

Thus far, microscopic theoretical studies on condensed Bose systems seem to have been carried out separately in two limiting cases with completely different approaches: (a) the weak-coupling regime where certain model Hamiltonians have been investigated based on the field theory;^{42,43} (b) the strong coupling regime where interests have been focused on describing superfluid ^4He quantitatively based on some variational wave functions,^{62,63,64} lattice-gas models which can be mapped onto spin systems,⁶⁵ and quantum Monte-Carlo calculations.⁶⁶ We hence need systematic investigations based on a model Hamiltonian from weak- to strong-coupling regimes, which may provide us more profound understanding on condensed Bose systems and shed a new light on the nature of the still mysterious lambda transition of superfluid ^4He .⁵⁰

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APPENDIX A: FEYNMAN RULES IN NAMBU SPACE

The bare perturbation expansion of the condensed Bose systems is usually carried out with respect to the condensate wave function $\Psi(\mathbf{r})$ and the non-interacting Green’s function:

$$G^{(0)}(\mathbf{r}_1\tau_1, \mathbf{r}_2\tau_2) \equiv -\langle T_\tau \phi(\mathbf{r}_1\tau_1) \phi^\dagger(\mathbf{r}_2\tau_2) \rangle_0. \quad (\text{A1})$$

The anomalous (i.e., off-diagonal) Green’s function is not necessary before the renormalization, and we have well-established Feynman rules for this purpose. We will show that the same rules can be used with a slight modification to the perturbation expansion in terms of the Nambu matrix of Eq. (3). This extension will be performed in exactly the same way as the extension from the normal to the superconducting Fermi systems.⁵⁵

Let us specifically consider the following term in the interaction:

$$H^{(3)} \equiv U_{11'} \left(\Psi_1^* \phi_1^\dagger \phi_{1'} \phi_1 + \phi_1^\dagger \phi_1^\dagger \phi_{1'} \Psi_1 \right), \quad (\text{A2})$$

where $U_{11'} \equiv \mathcal{U}(\mathbf{r}_1 - \mathbf{r}_{1'})$, $\phi_1 \equiv \phi(\mathbf{r}_1)$, etc., and summations over the repeated indices are implied. Using the normal-ordering operator N , we first rewrite Eq. (A2) as

$$H^{(3)} = \mathcal{U}_{11'} N \left(\Psi_1^* \phi_1 \phi_{1'}^\dagger + \phi_1^\dagger \Psi_1 \phi_{1'} \right). \quad (\text{A3a})$$

With the operator N in front, Eq. (A2) is further transformed into

$$H^{(3)} = \mathcal{U}_{11'} N \left(\frac{1}{2} \vec{\Psi}_1^\dagger \vec{\phi}_1 \frac{1}{2} \vec{\phi}_{1'}^\dagger \vec{\phi}_{1'} + \frac{1}{2} \vec{\phi}_1^\dagger \vec{\Psi}_1 \frac{1}{2} \vec{\phi}_{1'}^\dagger \vec{\phi}_{1'} \right), \quad (\text{A3b})$$

where $\vec{\phi}$ and $\vec{\Psi}$ are the spinors of Eq. (2). Comparing Eqs. (A3a) and (A3b), we observe the following correspondence:

$$\phi_1^\dagger \leftrightarrow \vec{\phi}_1^\dagger, \quad \Psi_1^* \leftrightarrow \vec{\Psi}_1^\dagger, \quad \phi_1^\dagger \phi_1 \leftrightarrow \frac{1}{2} \vec{\phi}_1^\dagger \vec{\phi}_1, \quad \text{etc.} \quad (\text{A4})$$

Let us perform a perturbation expansion in the imaginary time domain with respect to (A3b). We hence include τ_i in the index i , i.e., $i \equiv \mathbf{r}_i \tau_i$ and $i' \equiv \mathbf{r}_{i'} \tau_{i'}$. Consider an n th-order term in the expansion and take a contraction of $\vec{\phi}_i^\dagger$ with $\frac{1}{2} \vec{\phi}_j^\dagger \vec{\phi}_j$. We then find that $\vec{\phi}_i^\dagger$ and $\vec{\phi}_j$ in $\frac{1}{2} \vec{\phi}_j^\dagger \vec{\phi}_j$ contribute equivalently to the contraction, as shown easily by writing it down with respect to ϕ_i , ϕ_i^\dagger , ϕ_j , and ϕ_j^\dagger ; the statement is valid even if we formally retain the anomalous averages. Because of this fact, we can introduce the

rule: Contract $\vec{\phi}_i^\dagger$ only with $\vec{\phi}_j$ in $\frac{1}{2} \vec{\phi}_j^\dagger \vec{\phi}_j$ and multiply the contribution by 2. This yields $\vec{\phi}_j^\dagger \langle T_\tau N \vec{\phi}_j \vec{\phi}_i^\dagger \rangle_0$, where N is effective only when i and j belong to the same interaction line according to the definition in Eq. (A3). Note $\langle T_\tau \vec{\phi}_j \vec{\phi}_i^\dagger \rangle_0 = -\hat{\tau}_3 \hat{G}_{ji}^{(0)}$ as realized from Eq. (3). The rule allows us to perform a perturbation expansion in Nambu space by using only the Feynman diagrams for $G_{ij}^{(0)}$. The following two points should be supplemented: (a) A factor $\frac{1}{2}$ remains uncanceled for each closed particle line, due to the fact that we have to fix the starting pair $\frac{1}{2} \vec{\phi}_i^\dagger \vec{\phi}_i$ for each closed line. (b) The contraction of $\vec{\phi}_i$ with the last $\vec{\phi}_k^\dagger$ in the closed particle line may be transformed as

$$\frac{1}{2} \langle T_\tau N \vec{\phi}_k^\dagger \hat{A}_{ki} \vec{\phi}_i \rangle_0 = \frac{1}{2} \text{Tr} \hat{A}_{ki} \langle T_\tau N \vec{\phi}_i \vec{\phi}_k^\dagger \rangle_0, \quad (\text{A5})$$

where \hat{A}_{ki} is a Nambu matrix composed of the contractions connecting k with i . (c) As for the open line starting from $\frac{1}{2} \vec{\phi}_i^\dagger \vec{\Psi}_i$ and ending at $\frac{1}{2} \vec{\Psi}_k^\dagger \vec{\phi}_k$, the two factors $\frac{1}{2}$ remain uncanceled. These rules are valid even after including the interactions other than Eq. (A3).

In summary, we can carry out a perturbation expansion in Nambu space by modifying the Feynman rules for $G^{(0)}$, Ψ , and Ψ^* as follows: (i) $G_{ij}^{(0)} \rightarrow \hat{\tau}_3 \hat{G}_{ij}^{(0)}$, $\Psi_i \rightarrow \frac{1}{2} \vec{\Psi}_i$, and $\Psi_i^* \rightarrow \frac{1}{2} \vec{\Psi}_i^\dagger$; (ii) $\frac{1}{2} \text{Tr}$ for every closed particle line. Note that the operator N in $\langle T_\tau N \vec{\phi}_i \vec{\phi}_k^\dagger \rangle_0$ transforms into the matrix of Eq. (6) in the frequency space.

Let us write down the contributions of the diagrams in Fig. 1 based on the above rules with $\hat{G}^{(0)} \rightarrow \hat{G}$. This yields Φ_{HFB} . We then modify it slightly as described below Eq. (11a). We thereby obtain Φ of Eq. (11a).

APPENDIX B: CONSERVATION LAWS

It is shown that the Φ derivative approximation defined by Eqs. (7) and (10) automatically satisfies various conservation laws.

1. Definitions

Since we work in the real-time domain, we need modifications of various definitions. The Green’s function is now defined by

$$\hat{G}(1, 2) \equiv -\frac{i}{\hbar} \hat{\tau}_3 \langle T \vec{\phi}(1) \vec{\phi}^\dagger(2) \rangle, \quad (\text{B1})$$

with $1 \equiv \mathbf{r}_1 t_1$. It obeys the equation of motion:

$$i\hbar \frac{\partial \hat{G}(1, 1')}{\partial t_1} - \hat{\tau}_3 K_1 \hat{G}(1, 1') = \hat{1} \delta(1, 1') + \hat{\Sigma}(1, \bar{2}) \hat{G}(\bar{2}, 1'), \quad (\text{B2a})$$

or equivalently,

$$-i\hbar \frac{\partial \hat{G}(1, 1')}{\partial t_{1'}} - K_1 \hat{G}(1, 1') \hat{\tau}_3 = \hat{1} \delta(1, 1') + \hat{G}(1, \bar{2}) \hat{\Sigma}(\bar{2}, 1'). \quad (\text{B2b})$$

Here K_1 is given by Eq. (5), and integration over the barred index $\bar{2}$ is implied. Next, the condensate wave function satisfies

$$i\hbar \frac{\partial}{\partial t_1} \bar{\Psi}(1) - K_1 \hat{\tau}_3 \bar{\Psi}(1) = \hat{\tau}_3 \bar{\eta}(1), \quad (\text{B2c})$$

or equivalently,

$$-i\hbar \frac{\partial}{\partial t_1} \bar{\Psi}^\dagger(1) - K_1 \bar{\Psi}^\dagger(1) \hat{\tau}_3 = \bar{\eta}^\dagger(1) \hat{\tau}_3. \quad (\text{B2d})$$

Here $\bar{\Psi}$ is given in Eq. (2b), and $\bar{\eta}(1)$ denotes

$$\bar{\eta}(1) \equiv \begin{bmatrix} \eta(1) \\ \eta^*(1) \end{bmatrix}. \quad (\text{B3})$$

The key quantities in Eq. (B2) are $\hat{\Sigma}$ and η . In the Φ -derivative approximation²⁵ adopted here, they are determined from a functional $\Phi = \Phi(\hat{G}, \Psi, \Psi^*)$ by

$$\hat{\Sigma}(1, 1') = -2i \frac{\delta \Phi}{\delta \hat{G}(1', 1)}, \quad (\text{B4a})$$

$$\eta(1) = \hbar \frac{\delta \Phi}{\delta \Psi^*(1)}. \quad (\text{B4b})$$

Note that this Φ is different in definition from those of Baym⁴⁸ and Hohenberg and Martin²⁵ by factor i , i.e., $\Phi = i\Phi_{\text{Baym}} = i\Phi_{\text{HM}}$. The present definition has an advantage that Φ becomes real within the mean-field approximation. A comment is also necessary on Eq. (B1). When $t_2 = t_1$, the operator ϕ^\dagger in $\hat{G}(1, 2)$ should be placed to the left of ϕ by definition. This procedure is in accordance with the treatment on the equal-time operators in the calculation of Φ . Put it another way, the equal time implies $t_2 = t_{1+}$ for the (11) component of \hat{G} and $t_2 = t_{1-}$ for the (22) component. Thus, t_2 is not exactly equal to t_1 for the diagonal elements of \hat{G} .

2. Identities

With Eq. (B4), we can prove several identities by exactly following the argument of Baym.⁴⁸

Suppose we perform the gauge transformation:

$$\begin{cases} \hat{G}(1, 2) \rightarrow e^{i\chi(1)\hat{\tau}_3} \hat{G}(1, 2) e^{-i\chi(2)\hat{\tau}_3} \\ \Psi(1) \rightarrow e^{i\chi(1)} \Psi(1) \end{cases}, \quad (\text{B5})$$

where $\chi(1)$ is an arbitrary real function. The corresponding variations in \hat{G} and Ψ are given to the leading order by

$$\begin{cases} \delta \hat{G}(1, 2) = i[\chi(1)\hat{\tau}_3 \hat{G}(1, 2) - \hat{G}(1, 2)\chi(2)\hat{\tau}_3] \\ \delta \Psi(1) = i\chi(1)\Psi(1) \end{cases}, \quad (\text{B6})$$

respectively. However, Φ is clearly invariant under Eq. (B5), i.e., $\delta\Phi = 0$. This yields

$$\frac{i\hbar}{2} \text{Tr} \Sigma(\bar{1}, \bar{2}) \delta \hat{G}(\bar{2}, \bar{1}) + \delta \Psi^*(\bar{1}) \eta(\bar{1}) + \delta \Psi(\bar{1}) \eta^*(\bar{1}) = 0. \quad (\text{B7})$$

Substituting Eq. (B6) into Eq. (B7) and recalling $\chi(1)$ is arbitrary, we obtain

$$\frac{1}{2} \text{Tr} \hat{\tau}_3 [\hat{\Sigma}(1, \bar{2}) \hat{G}(\bar{2}, 1) - \hat{G}(1, \bar{2}) \hat{\Sigma}(\bar{2}, 1)] - \frac{i}{\hbar} \bar{\Psi}^\dagger(1) \hat{\tau}_3 \bar{\eta}(1) = 0, \quad (\text{B8})$$

with $\bar{\Psi}^\dagger \equiv (\Psi^* \Psi)$.

We next consider the Galilean transformation:

$$\begin{cases} \hat{G}(1, 2) \rightarrow \hat{G}(\mathbf{r}_1 + \mathbf{R}(t_1), t_1; \mathbf{r}_2 + \mathbf{R}(t_2), t_2) \\ \Psi(1) \rightarrow \Psi(\mathbf{r}_1 + \mathbf{R}(t_1), t_1) \end{cases}. \quad (\text{B9})$$

The corresponding leading-order variations in \hat{G} and Ψ are given by

$$\begin{cases} \delta \hat{G}(1, 2) = [\mathbf{R}(t_1) \cdot \nabla_1 + \mathbf{R}(t_2) \cdot \nabla_2] \hat{G}(1, 2) \\ \delta \Psi(1) = \mathbf{R}(t_1) \cdot \nabla_1 \Psi(1) \end{cases}. \quad (\text{B10})$$

However, Φ remains invariant since it is a quantity obtained by integrations over all the space-time variables. We hence conclude that Eq. (B7) holds also in this case. Substituting Eq. (B10) into Eq. (B7) and recalling $\mathbf{R}(t)$ is arbitrary, we obtain

$$\int \mathbf{S}(1) d\mathbf{r}_1 = \mathbf{0}, \quad (\text{B11})$$

with

$$\begin{aligned} \mathbf{S}(1) \equiv & \frac{1}{4} (\nabla_1 - \nabla_{1'}) \{ i\hbar \text{Tr} [\hat{G}(1, \bar{2}) \hat{\Sigma}(\bar{2}, 1') - \hat{\Sigma}(1, \bar{2}) \\ & \times \hat{G}(\bar{2}, 1')] - 2\bar{\Psi}^\dagger(1') \bar{\eta}(1) \} \big|_{1'=1}. \end{aligned} \quad (\text{B12})$$

Here terms with $\nabla_1 \hat{\Sigma}(1, 2)$ and $\nabla_1 \bar{\eta}(1)$ have been obtained through integrations by parts.

We finally consider the “rubber-clock” transformation of Baym:⁴⁸ $t \rightarrow \theta(t) \equiv t + f(t)$ with $f(\pm\infty) = 0$. It yields

$$\begin{cases} \hat{G}(1, 2) \rightarrow \left(\frac{d\theta_1}{dt_1} \right)^{1/4} \hat{G}(\mathbf{r}_1 \theta_1, \mathbf{r}_2 \theta_2) \left(\frac{d\theta_2}{dt_2} \right)^{1/4} \\ \Psi(1) \rightarrow \left(\frac{d\theta_1}{dt_1} \right)^{1/4} \Psi(\mathbf{r}_1 \theta_1) \end{cases}. \quad (\text{B13})$$

The factor $(d\theta/dt)^{1/4}$ compensates the Jacobian for $t \rightarrow \theta$, thereby making the integration of $H_{\text{int}}(t)$ over t invariant in form through the change of variables. The corresponding leading-order variations in \hat{G} and Ψ are given by

$$\begin{cases} \delta \hat{G}(1, 2) = \left(\frac{f'_1 + f'_2}{4} + f_1 \frac{\partial}{\partial t_1} + f_2 \frac{\partial}{\partial t_2} \right) \hat{G}(1, 2) \\ \delta \Psi(1) = \left(\frac{f'_1}{4} + f_1 \frac{\partial}{\partial t_1} \right) \Psi(1) \end{cases}, \quad (\text{B14})$$

with $f_j \equiv f(t_j)$. However, Φ remains invariant. Hence Eq. (B7) holds also in this case. Substituting Eq. (B14) into Eq. (B7) and recalling $f(t)$ is arbitrary, we obtain the third identity:

$$\frac{d\langle H_{\text{int}} \rangle_1}{dt_1} = \frac{1}{2} \int d\mathbf{r}_1 \frac{\partial}{\partial t_1} \{ i\hbar \text{Tr} [\hat{G}(1, \bar{2}) \hat{\Sigma}(\bar{2}, 1') + \hat{\Sigma}(1', \bar{2}) \times \hat{G}(\bar{2}, 1)] + \bar{\Psi}^\dagger(1) \bar{\eta}(1') + \bar{\eta}^\dagger(1') \bar{\Psi}(1) \} \Big|_{1'=1}, \quad (\text{B15})$$

where $\langle H_{\text{int}} \rangle_1$ is defined by

$$\langle H_{\text{int}} \rangle_1 = \frac{1}{8} \int d\mathbf{r}_1 \{ i\hbar \text{Tr} [\hat{G}(1, \bar{2}) \hat{\Sigma}(\bar{2}, 1) + \hat{\Sigma}(1, \bar{2}) \hat{G}(\bar{2}, 1)] + \bar{\Psi}^\dagger(1) \bar{\eta}(1) + \bar{\eta}^\dagger(1) \bar{\Psi}(1) \}. \quad (\text{B16})$$

Equation (B16) indeed corresponds to the interaction energy of the system. This can be checked as follows: (i) write down the equations of motion for ϕ and Ψ in terms of the field operators and the condensate wave function; (ii) construct the interaction energy by adding those equations appropriately; and (iii) transform the one-particle energy in the equation by using Eq. (B2).

Equations (B8), (B11), and (B15) are the basic identities to be used below.

3. Conservation laws

Let us operate $\frac{1}{2} \text{Tr} \hat{\tau}_3$, $-\frac{1}{2} \text{Tr} \hat{\tau}_3$, and $-\frac{i}{\hbar} \bar{\Psi}^\dagger(1)$ to Eqs. (B2a), (B2b), and (B2c), respectively. Adding the resulting three equations, setting $1' = 1$, and noting Eq. (B8), we obtain the particle conservation law as

$$\frac{\partial n(1)}{\partial t_1} + \nabla_1 \mathbf{j}(1) = 0, \quad (\text{B17})$$

where $n(1)$ and $\mathbf{j}(1)$ are defined by

$$n(1) = \rho(1, 1), \quad (\text{B18})$$

$$\mathbf{j}(1) = \frac{-i\hbar}{2m} (\nabla_1 - \nabla_{1'}) \rho(1, 1') \Big|_{1'=1}, \quad (\text{B19})$$

with

$$\rho(1, 1') \equiv \langle \phi^\dagger(1') \phi(1) \rangle + \Psi(1) \Psi^*(1'). \quad (\text{B20})$$

This $\rho(1, 1')$ is the one-body density matrix appearing in the evaluation of every one-particle operator.

To obtain the momentum conservation law, we operate $-\frac{i\hbar}{4m} \text{Tr} (\nabla_1 - \nabla_{1'})$, $\frac{i\hbar}{4m} \text{Tr} (\nabla_1 - \nabla_{1'})$, and $-\frac{1}{2m} \bar{\Psi}^\dagger(1) \hat{\tau}_3 \nabla_1$ to Eqs. (B2a), (B2b), and (B2c), respectively. We also multiply Eq. (B2d) from the right by $\frac{1}{2m} \hat{\tau}_3 \nabla_1 \bar{\Psi}(1)$. Adding the four equations and setting $1' = 1$, we obtain

$$\frac{\partial}{\partial t_1} \mathbf{j}(1) + \frac{n(1)}{m} \nabla_1 V(1) + \frac{1}{m} \nabla_1 \cdot \mathbf{\Pi}(1) = \frac{1}{m} \mathbf{S}(1). \quad (\text{B21})$$

Here $\mathbf{j}(1)$, $n(1)$, and $\mathbf{S}(1)$ are given by Eqs. (B19), (B18), and (B12), respectively, and $\mathbf{\Pi}(1)$ is a tensor defined by

$$\Pi_{\alpha\beta}(1) = -\frac{\hbar^2}{4m} (\nabla_{1\alpha} - \nabla_{1'\alpha}) (\nabla_{1\beta} - \nabla_{1'\beta}) \rho(1, 1') \Big|_{1'=1}. \quad (\text{B22})$$

Integrating Eq. (B21) over \mathbf{r}_1 and noting Eq. (B11), we obtain the conservation law for the total momentum as

$$\frac{\partial}{\partial t_1} \int \mathbf{j}(1) d\mathbf{r}_1 = -\frac{1}{m} \int n(1) \nabla_1 V(1) d\mathbf{r}_1. \quad (\text{B23})$$

We finally consider the energy conservation law. The time derivative of the interaction energy is given by Eq. (B15). The terms in the curly bracket of Eq. (B15) can be transformed into an expression of using the left-hand sides of Eq. (B2). We then find that the terms with the operator $i\hbar \frac{\partial}{\partial t_{1'}}$ cancels out upon applying $\frac{\partial}{\partial t_1}$ in front of the curly bracket. We thereby obtain

$$\frac{d\langle H_{\text{int}} \rangle_1}{dt_1} = - \int d\mathbf{r}_1 K_1 \frac{\partial}{\partial t_1} \rho(\mathbf{r}_1 t_1, \mathbf{r}'_1 t_1) \Big|_{\mathbf{r}'_1 = \mathbf{r}_1}, \quad (\text{B24})$$

with $\rho(1, 1')$ defined by Eq. (B20). When K has no time dependence as given by Eq. (5), Eq. (B24) directly leads to $\langle K + H_{\text{int}} \rangle = \text{constant}$. Following Kadanoff and Baym,⁶⁷ we may alternatively consider V as a small time-dependent external field and trace the time variation of the internal energy $\langle K^{(0)} + H_{\text{int}} \rangle$, where $K^{(0)} \equiv -\frac{\hbar^2}{2m} \nabla^2$. Using Eq. (B17) and performing integration by parts with respect to \mathbf{r}_1 , we obtain

$$\frac{d\langle K^{(0)} + H_{\text{int}} \rangle_1}{dt_1} = - \int \mathbf{j}(1) \cdot \nabla_1 V(1) d\mathbf{r}_1. \quad (\text{B25})$$

Thus, we have seen that the conservation laws are automatically obeyed as Eq. (B17), (B23), and (B25) in the Φ derivative approximation of Eq. (B4).

APPENDIX C: THE IRK THEORY

It will be shown that the thermodynamic functional presented by Ivanov, Riek, and Knoll⁵¹ (IRK) leads to exactly the same thermodynamic properties for the weakly interacting Bose gases as the present theory.

The IRK self-energy $\hat{\Sigma}^{(\text{IRK})}$ is calculated from Eq. (12) by Eq. (7). The result can be written as

$$\hat{\Sigma}^{(\text{IRK})}(\mathbf{r}, \mathbf{r}') = \begin{bmatrix} \Sigma(\mathbf{r}, \mathbf{r}') & -\Delta^{(\text{IRK})}(\mathbf{r}, \mathbf{r}') \\ \Delta^{(\text{IRK})*}(\mathbf{r}, \mathbf{r}') & -\Sigma^*(\mathbf{r}, \mathbf{r}') \end{bmatrix}, \quad (\text{C1})$$

where Σ is given by Eq. (14a), and $\Delta^{(\text{IRK})}$ denotes

$$\Delta^{(\text{IRK})}(\mathbf{r}, \mathbf{r}') = \mathcal{U}(\mathbf{r} - \mathbf{r}') \tilde{\rho}^{(\text{IRK})}(\mathbf{r}, \mathbf{r}'), \quad (\text{C2})$$

with

$$\tilde{\rho}^{(\text{IRK})}(\mathbf{r}, \mathbf{r}') = \Psi(\mathbf{r}) \Psi(\mathbf{r}') - \langle \phi(\mathbf{r}) \phi(\mathbf{r}') \rangle^{(\text{IRK})}. \quad (\text{C3})$$

The minus sign in front of $\Delta^{(\text{IRK})}$ in Eq. (C1) has been introduced to make the coefficient $\Delta_{\mathbf{k}}^{(\text{IRK})}$ for the homogeneous system positive at low temperatures, in accordance with the definition of Δ in Eq. (14b). Next, the equation for $\Psi(\mathbf{r})$ is obtained from the thermodynamic functional Ω^{IRK} by $\partial\Omega^{\text{IRK}}/\partial\Psi(\mathbf{r})=0$. It is given by Eq. (16) with the replacement: $\Delta \rightarrow \Delta^{(\text{IRK})}$.

In a way parallel to Eqs. (18) and (24), let us introduce the Hamiltonian:

$$\hat{H}^{(\text{IRK})}(\mathbf{r}, \mathbf{r}') \equiv \hat{\tau}_3 K \delta(\mathbf{r} - \mathbf{r}') + \hat{\Sigma}^{(\text{IRK})}(\mathbf{r}, \mathbf{r}'), \quad (\text{C4})$$

and construct the eigenvalue problem as

$$\int \hat{H}^{(\text{IRK})}(\mathbf{r}, \mathbf{r}') \hat{u}_{\nu}^{(\text{IRK})}(\mathbf{r}') d\mathbf{r}' = \hat{u}_{\nu}^{(\text{IRK})}(\mathbf{r}) E_{\nu} \hat{\tau}_3, \quad (\text{C5})$$

where $\hat{u}_{\nu}^{(\text{IRK})}$ is defined by

$$\hat{u}_{\nu}^{(\text{IRK})}(\mathbf{r}) = \begin{bmatrix} u_{\nu}(\mathbf{r}) & v_{\nu}(\mathbf{r}) \\ v_{\nu}^*(\mathbf{r}) & u_{\nu}^*(\mathbf{r}) \end{bmatrix}. \quad (\text{C6})$$

The sign of $v_{\nu}^*(\mathbf{r})$ is chosen so that the coefficient $v_{\mathbf{k}}$ of the homogeneous system is positive, in accordance with the definition of $v_{\nu}^*(\mathbf{r})$ in Eq. (25a). The corresponding Green's function \hat{G}^{IRK} is obtained from Eq. (29) with the replacement $\hat{u}_{\nu} \rightarrow \hat{u}_{\nu}^{(\text{IRK})}$. Noting Eq. (30b) and the difference between Eqs. (25a) and (C6), we now conclude that $\langle \phi(\mathbf{r}) \phi(\mathbf{r}') \rangle^{(\text{IRK})}$ in Eq. (C3) satisfies $-\langle \phi(\mathbf{r}) \phi(\mathbf{r}') \rangle^{(\text{IRK})} = \langle \phi(\mathbf{r}) \phi(\mathbf{r}') \rangle$, which implies $\Delta^{(\text{IRK})} = \Delta$. Thus, the equations to determine the equilibrium are exactly the same between the present theory and the IRK theory. Finally, one can show that the equilibrium thermodynamic potential of the IRK theory is also given by Eq. (31). Thus, the two functionals (11a) and (12) yield exactly the same thermodynamic properties on BEC.

APPENDIX D: NON-HERMITIAN EIGENVALUE PROBLEM

In this Appendix we study possible origins of the non-Hermitian eigenvalue problem in BEC. It is shown that we have to treat the non-Hermitian matrix of Eq. (24) necessarily if we impose the two requirements: (i) the quasiparticle field obey the Bose statistics; (ii) the quasiparticle eigenstates be obtained by diagonalizing a matrix.

Let us introduce the quasiparticle field γ_{ν} through

$$\begin{bmatrix} \phi_{\mathbf{r}} \\ -\phi_{\mathbf{r}}^{\dagger} \end{bmatrix} = \sum_{\nu} \begin{bmatrix} u_{\nu} & -v_{\nu} \\ -v_{\nu}^* & u_{\nu}^* \end{bmatrix} \begin{bmatrix} \gamma_{\nu} \\ -\gamma_{\nu}^{\dagger} \end{bmatrix}, \quad (\text{D1})$$

where ν distinguishes quasiparticle eigenstates, and $\phi_{\mathbf{r}} = \phi(\mathbf{r})$, $u_{\nu} = u_{\nu}(\mathbf{r})$, etc. Equation (D1) may be written symbolically in a compact form as

$$\vec{\phi} = \hat{u} \vec{\gamma}, \quad (\text{D2})$$

where

$$\vec{\phi} \equiv \begin{bmatrix} \phi_{\mathbf{r}} \\ \phi_{\mathbf{r}'} \\ \vdots \\ -\phi_{\mathbf{r}}^{\dagger} \\ -\phi_{\mathbf{r}'}^{\dagger} \\ \vdots \end{bmatrix}, \quad \hat{u} \equiv \begin{bmatrix} \underline{u} & -\underline{v} \\ -\underline{v}^* & \underline{u}^* \end{bmatrix}, \quad \vec{\gamma} \equiv \begin{bmatrix} \gamma_{\nu} \\ \gamma_{\nu'} \\ \vdots \\ -\gamma_{\nu}^{\dagger} \\ -\gamma_{\nu'}^{\dagger} \\ \vdots \end{bmatrix}, \quad (\text{D3})$$

with

$$(\underline{u})_{\mathbf{r}\nu} = u_{\mathbf{r}\nu}, \quad (\underline{v})_{\mathbf{r}\nu} = v_{\mathbf{r}\nu}. \quad (\text{D4})$$

We now impose the condition that γ_{ν} as well as $\phi_{\mathbf{r}}$ obey the Bose statistics. This implies

$$\hat{\tau}_3 = [\vec{\phi}, \vec{\phi}^{\dagger}] = \hat{u} [\vec{\gamma}, \vec{\gamma}^{\dagger}] \hat{u}^{\dagger} = \hat{u} \hat{\tau}_3 \hat{u}^{\dagger}, \quad (\text{D5})$$

where $\hat{\tau}_3$ is an infinite matrix defined by

$$\hat{\tau}_3 \equiv \begin{bmatrix} \underline{1} & \underline{0} \\ \underline{0} & -\underline{1} \end{bmatrix}, \quad (\text{D6})$$

with $\underline{1}$ and $\underline{0}$ denoting the unit and the zero matrices, respectively. We also require that \hat{u} be composed of eigenstates of a matrix \hat{E} as

$$\hat{H} \hat{u} = \hat{u} \hat{E}, \quad (\text{D7})$$

where \hat{E} is a real diagonal matrix. Multiplying Eq. (D7) by $\hat{u}^{-1} = \hat{\tau}_3 \hat{u}^{\dagger} \hat{\tau}_3$ from the left, we obtain

$$\hat{\tau}_3 \hat{u}^{\dagger} \hat{\tau}_3 \hat{H} \hat{u} = \hat{E}. \quad (\text{D8a})$$

We next take the Hermitian conjugate of Eq. (D8a) and multiply the resulting equation by $\hat{\tau}_3$ from both sides; this yields

$$\hat{\tau}_3 \hat{u}^{\dagger} \hat{H}^{\dagger} \hat{\tau}_3 \hat{u} = \hat{E}. \quad (\text{D8b})$$

Subtracting Eq. (D8b) from Eq. (D8a) and multiplying the resulting equation by $\hat{\tau}_3 \hat{u}$ and $\hat{\tau}_3 \hat{u}^{\dagger}$ from the left and the right, respectively, we obtain

$$\hat{H}^{\dagger} = \hat{\tau}_3 \hat{H} \hat{\tau}_3. \quad (\text{D9})$$

Thus, \hat{H} is necessarily non-Hermitian with the property (D9).

APPENDIX E: DERIVING EQS. (31) AND (32)

We here derive expressions of the equilibrium thermodynamic potential (31) and the entropy (32).

Using Eqs. (18) and (28), the logarithmic term in Eq. (4) can be transformed as

$$\begin{aligned} L &\equiv \frac{T}{2} \sum_n \text{Tr} \hat{1}(z_n) \ln(\hat{\tau}_3 K + \hat{\Sigma} - z_n \hat{1}) \\ &= \frac{1}{2} \int d\mathbf{r} \int_C \frac{dz}{2\pi i} e^{z0_+} n(z) \sum_{\nu} \{ |u_{\nu}(\mathbf{r})|^2 [\ln(E_{\nu} - z) \\ &\quad + \ln(z - E_{\nu})] - |v_{\nu}(\mathbf{r})|^2 [\ln(E_{\nu} + z) + \ln(-z - E_{\nu})] \}, \end{aligned} \quad (\text{E1})$$

with $n(z) \equiv 1/(e^{z/T} - 1)$. Here we have used the standard procedure to change the summation over n into a contour integral⁶⁸ with the replacements $e^{zn_{0+}} \rightarrow n(z)e^{z_{0+}}$ and $e^{-zn_{0+}} \rightarrow -n(-z)e^{-z_{0+}}$ in the matrix $\hat{1}(z_n)$ of Eq. (6). Contour C consists of two parallel lines running along the imaginary axis as shown in Fig. 25.4 of Ref. 68, which can be deformed into contour C' in the same figure along the real axis. Performing integration by parts in terms of z and collecting residues within C' , we obtain

$$L = \sum_{\nu} \left[T \ln(1 - e^{-E_{\nu}/T}) - E_{\nu} \int |v_{\nu}(\mathbf{r})|^2 d\mathbf{r} \right]. \quad (\text{E2})$$

Next, we rewrite Φ of Eq. (11a) by using Eqs. (13)-(15) as

$$\Phi = \frac{1}{4} \text{Tr} \int d\mathbf{r} \int d\mathbf{r}' \hat{\Sigma}(\mathbf{r}, \mathbf{r}') \left[-T \sum_n \hat{G}(\mathbf{r}', \mathbf{r}; z_n) \hat{1}(z_n) + \hat{\tau}_3 \vec{\Psi}(\mathbf{r}') \vec{\Psi}^{\dagger}(\mathbf{r}) \right]. \quad (\text{E3})$$

Finally, the first integral in Eq. (4) is transformed with Eq. (16) into an expression without K . Substituting the result together with Eqs. (E2) and (E3) into Eq. (4), we arrive at Eq. (31).

We next derive Eq. (32) by closely following the procedure of Ref. 69. We first transform all the summations over n in Eq. (4) into contour integrals of using $n(z)$. With the properties $\delta\Omega/\delta\Psi^* = 0$ and $\delta\Omega/\delta\hat{G} = \hat{0}$, the differentiation $-\partial\Omega/\partial T$ need be carried out only with respect to the explicit T dependence in $n(z)$. The term from Φ cancels that from the second term in the square bracket of Eq. (4). The remaining term is L of Eq. (E1), whose explicit T dependence is transformed into the first term in Eq. (E2). We hence obtain Eq. (32).

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